



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:54 pm BST

PDB ID : 4ZH2
Title : Crystal structure of Escherichia coli RNA polymerase in complex with CBR703
Authors : Feng, Y.; Ebright, R.H.
Deposited on : 2015-04-24
Resolution : 4.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

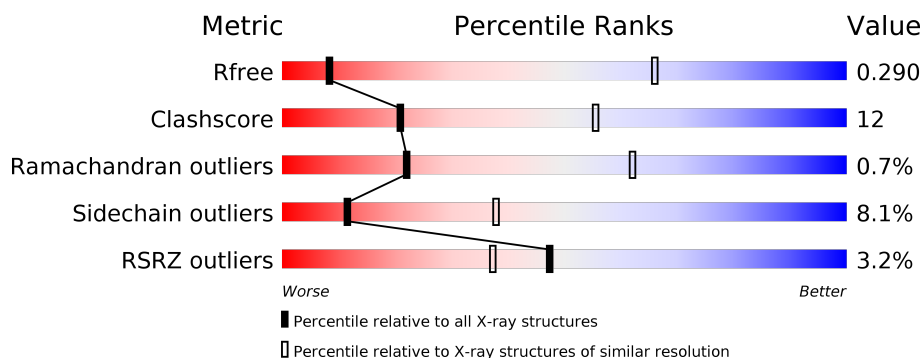
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1005 (4.62-3.78)
Clashscore	141614	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)
RSRZ outliers	127900	1063 (4.70-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	335	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>25%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	335	<div> <div>2%</div> <div> <div></div> <div>39%</div> <div>24%</div> <div>•</div> <div>36%</div> </div> </div>
1	G	335	<div> <div>0%</div> <div> <div></div> <div>41%</div> <div>24%</div> <div>•</div> <div>33%</div> </div> </div>
1	H	335	<div> <div>2%</div> <div> <div></div> <div>42%</div> <div>20%</div> <div>••</div> <div>36%</div> </div> </div>
2	C	1342	<div> <div>2%</div> <div> <div></div> <div>68%</div> <div>30%</div> <div>•</div> </div> </div>
2	I	1342	<div> <div>4%</div> <div> <div></div> <div>68%</div> <div>30%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	D	1407	
3	J	1407	
4	E	91	
4	K	91	
5	F	613	
5	L	613	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	4OB	C	2001	-	-	X	-
6	4OB	I	2001	-	-	X	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 57763 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	0
			2328	1456	413	451	8			
1	B	216	Total	C	N	O	S	0	0	0
			1667	1041	294	326	6			
1	G	224	Total	C	N	O	S	0	0	0
			1730	1076	308	340	6			
1	H	216	Total	C	N	O	S	0	0	0
			1662	1038	292	326	6			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	expression tag	UNP P0A7Z4
A	-4	HIS	-	expression tag	UNP P0A7Z4
A	-3	HIS	-	expression tag	UNP P0A7Z4
A	-2	HIS	-	expression tag	UNP P0A7Z4
A	-1	HIS	-	expression tag	UNP P0A7Z4
A	0	HIS	-	expression tag	UNP P0A7Z4
A	1	HIS	-	expression tag	UNP P0A7Z4
B	-5	MET	-	expression tag	UNP P0A7Z4
B	-4	HIS	-	expression tag	UNP P0A7Z4
B	-3	HIS	-	expression tag	UNP P0A7Z4
B	-2	HIS	-	expression tag	UNP P0A7Z4
B	-1	HIS	-	expression tag	UNP P0A7Z4
B	0	HIS	-	expression tag	UNP P0A7Z4
B	1	HIS	-	expression tag	UNP P0A7Z4
G	-5	MET	-	expression tag	UNP P0A7Z4
G	-4	HIS	-	expression tag	UNP P0A7Z4
G	-3	HIS	-	expression tag	UNP P0A7Z4
G	-2	HIS	-	expression tag	UNP P0A7Z4
G	-1	HIS	-	expression tag	UNP P0A7Z4
G	0	HIS	-	expression tag	UNP P0A7Z4
G	1	HIS	-	expression tag	UNP P0A7Z4

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-5	MET	-	expression tag	UNP P0A7Z4
H	-4	HIS	-	expression tag	UNP P0A7Z4
H	-3	HIS	-	expression tag	UNP P0A7Z4
H	-2	HIS	-	expression tag	UNP P0A7Z4
H	-1	HIS	-	expression tag	UNP P0A7Z4
H	0	HIS	-	expression tag	UNP P0A7Z4
H	1	HIS	-	expression tag	UNP P0A7Z4

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0	0
			10570	6631	1841	2055	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10566	6629	1840	2054	43			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1166	Total	C	N	O	S	0	0	0
			9107	5723	1634	1704	46			
3	J	1334	Total	C	N	O	S	0	0	0
			10369	6513	1850	1957	49			

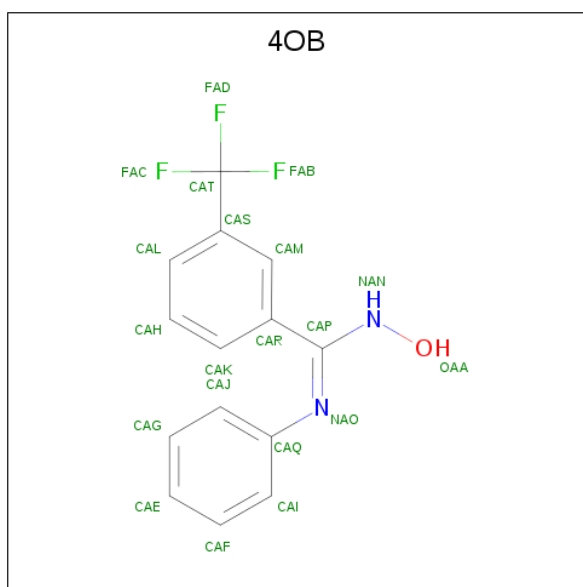
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	542	Total	C	N	O	S	0	0	0
			4204	2625	752	801	26			
5	L	539	Total	C	N	O	S	0	0	0
			4196	2619	749	802	26			

- Molecule 6 is N-hydroxy-N'-phenyl-3-(trifluoromethyl)benzenecarboximidamide (three-letter code: 4OB) (formula: C₁₄H₁₁F₃N₂O).



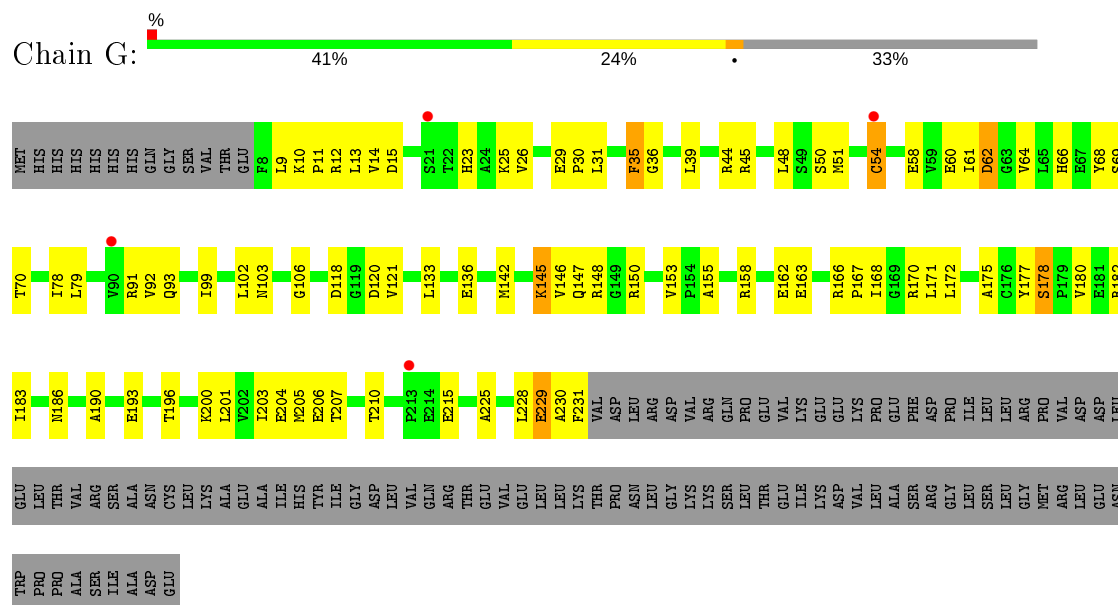
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	F	N	O	0	0
			20	14	3	2	1		
6	I	1	Total	C	F	N	O	0	0
			20	14	3	2	1		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

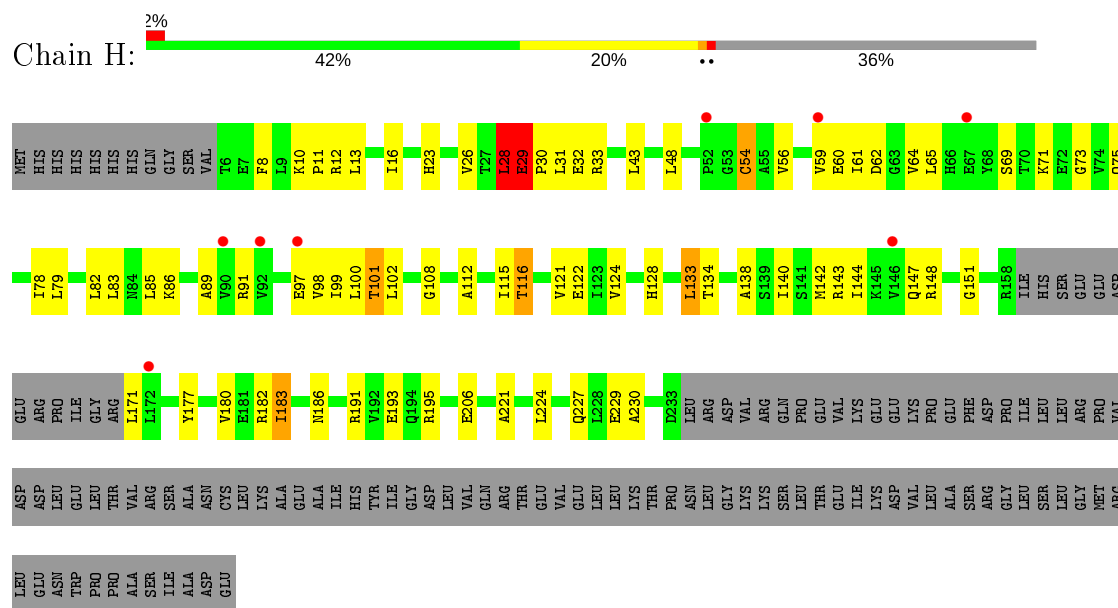
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

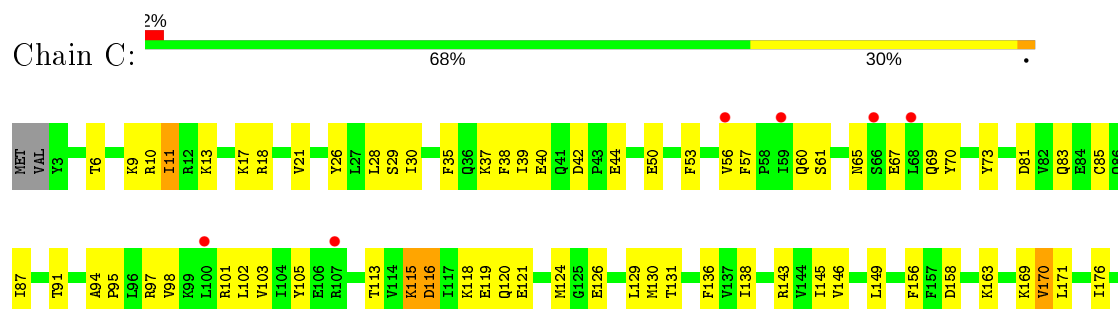
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	2	Total	Zn	0	0
			2	2		
8	D	2	Total	Zn	0	0
			2	2		

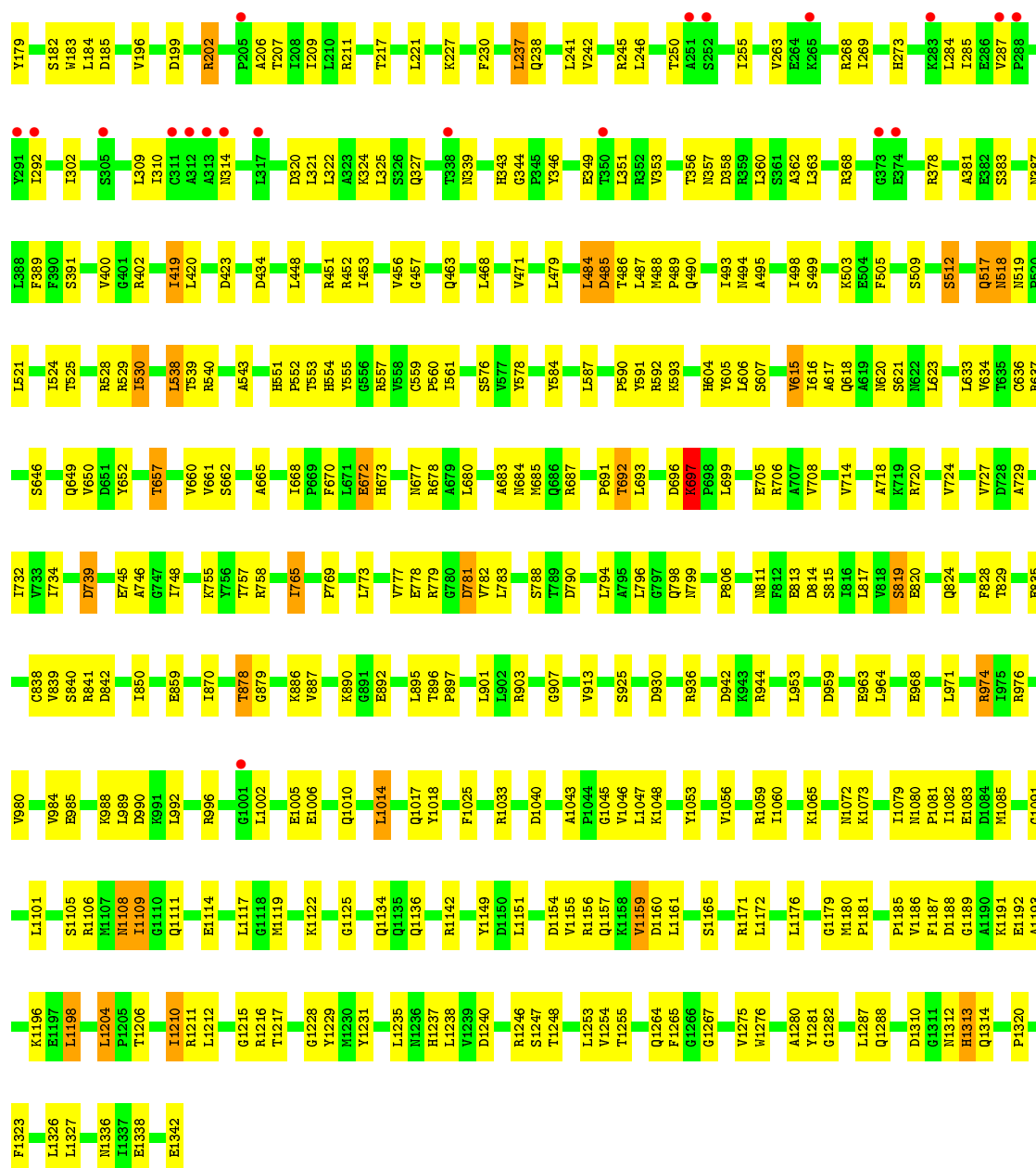


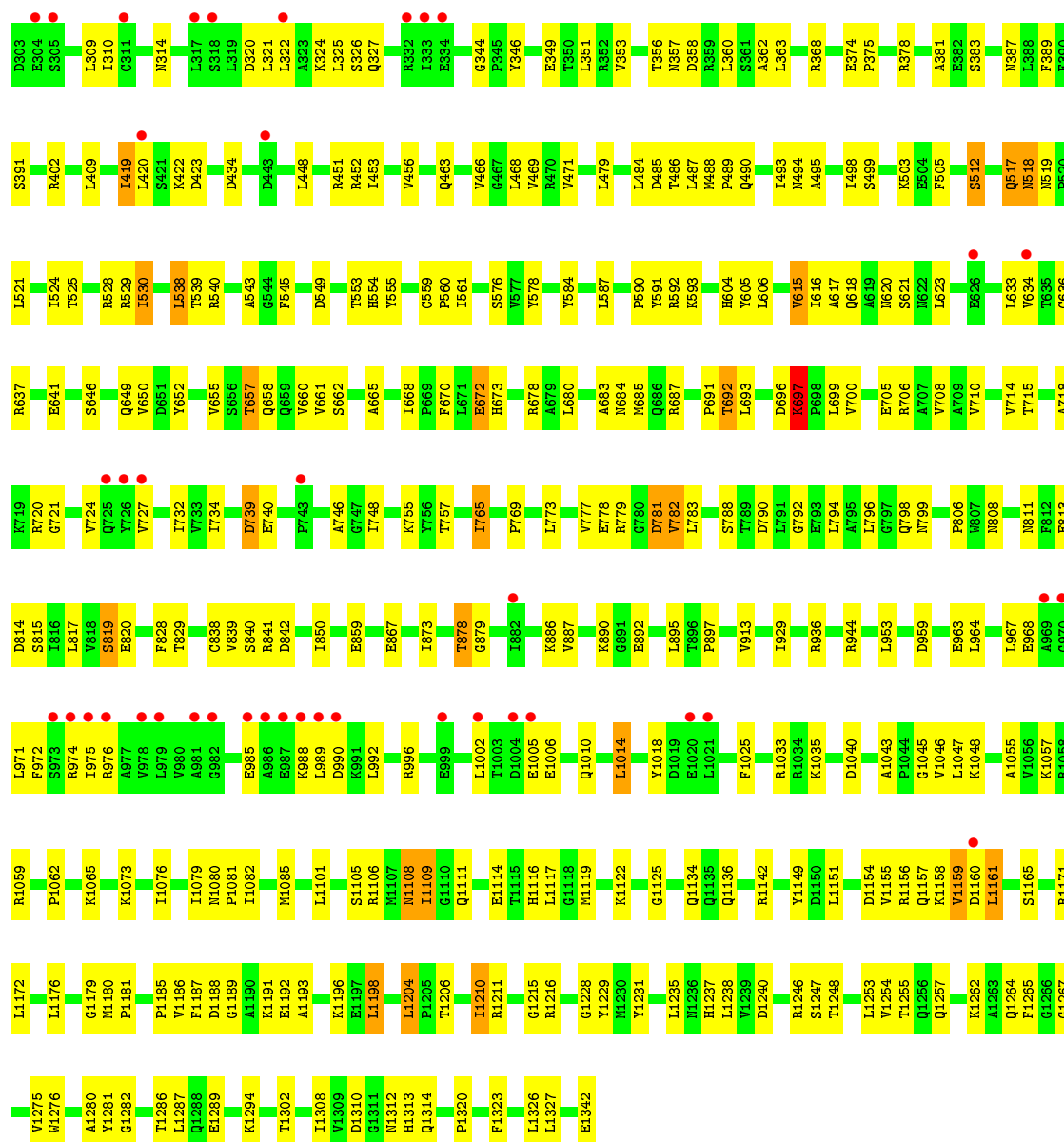
• Molecule 1: DNA-directed RNA polymerase subunit alpha



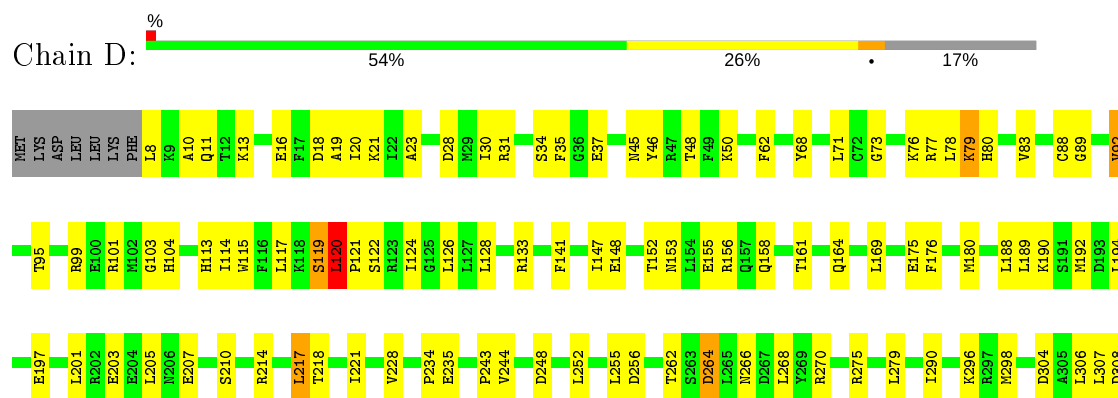
• Molecule 2: DNA-directed RNA polymerase subunit beta

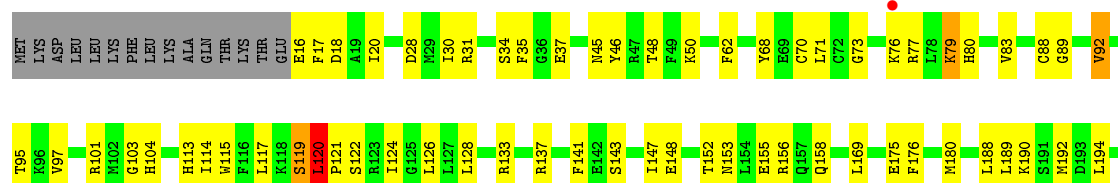


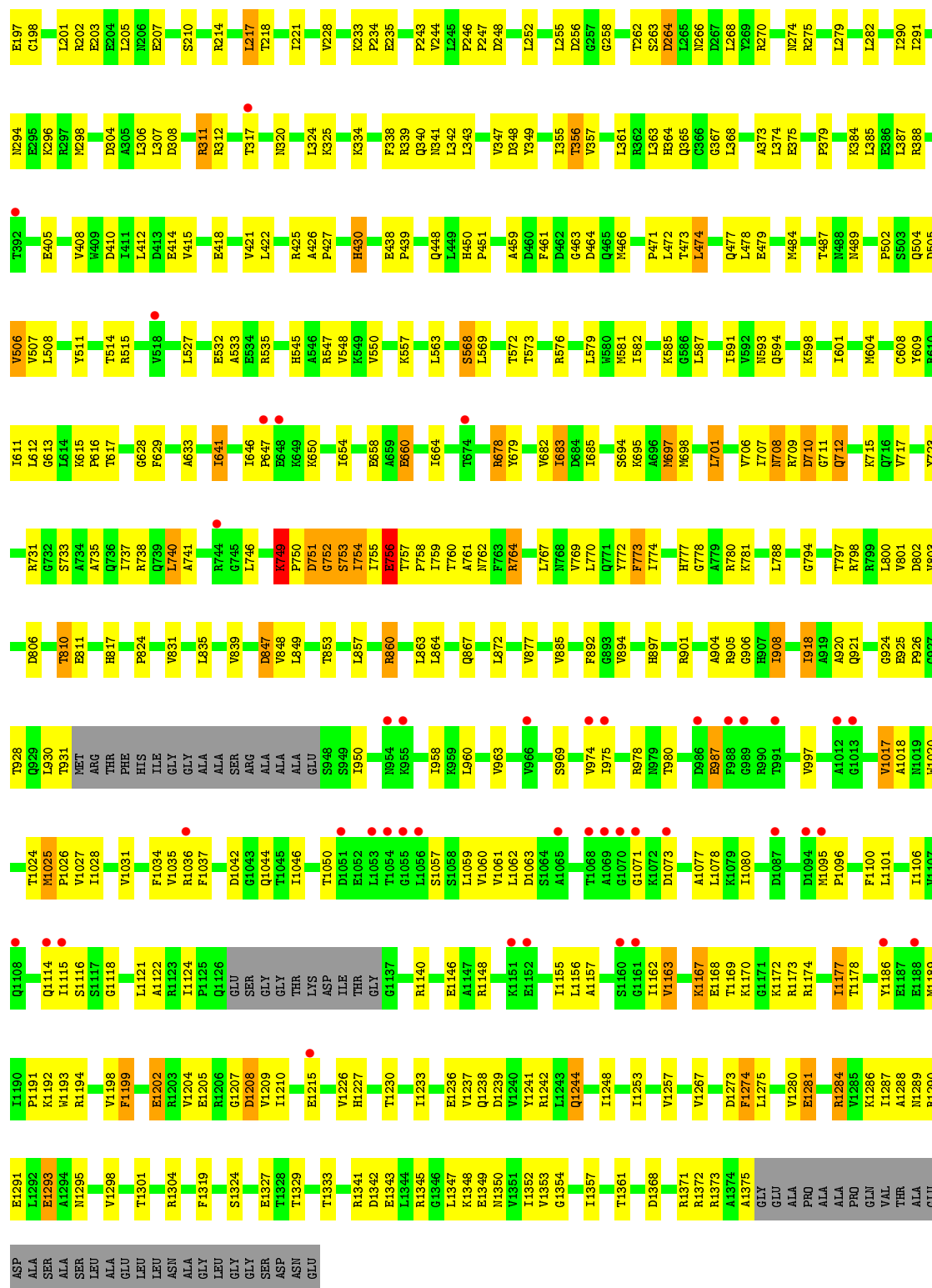




- Molecule 3: DNA-directed RNA polymerase subunit beta'

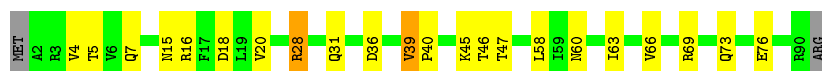






- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 74% 22%



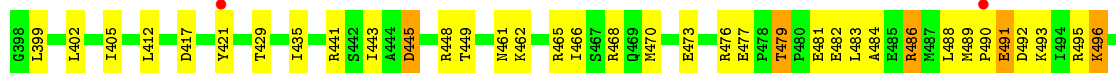
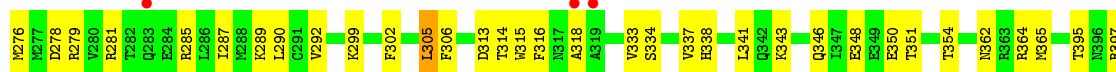
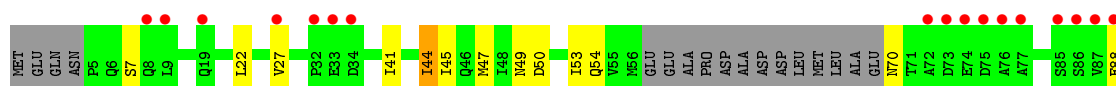
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain K: 63% 22% 13%



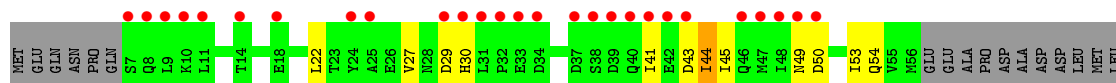
- Molecule 5: RNA polymerase sigma factor RpoD

Chain F: 6% 64% 22% 12%



- Molecule 5: RNA polymerase sigma factor RpoD

Chain L: 6% 62% 24% 12%





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	185.79 Å 205.83 Å 307.46 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.76 – 4.20 49.75 – 4.20	Depositor EDS
% Data completeness (in resolution range)	94.5 (49.76-4.20) 93.8 (49.75-4.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 4.14 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.266 , 0.288 0.267 , 0.290	Depositor DCC
R_{free} test set	2581 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	152.4	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 99.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	57763	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4OB, ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.29	0/2358	0.61	1/3197 (0.0%)
1	B	0.33	0/1687	0.64	0/2286
1	G	0.29	0/1751	0.63	0/2373
1	H	0.30	0/1681	0.67	3/2278 (0.1%)
2	C	0.24	0/10739	0.46	0/14489
2	I	0.23	0/10735	0.45	0/14484
3	D	0.25	0/9246	0.47	1/12478 (0.0%)
3	J	0.24	0/10525	0.46	1/14212 (0.0%)
4	E	0.23	0/693	0.45	0/935
4	K	0.22	0/629	0.45	0/847
5	F	0.25	0/4254	0.47	0/5731
5	L	0.25	0/4246	0.47	0/5720
All	All	0.25	0/58544	0.49	6/79030 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1
3	J	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	ARG	NE-CZ-NH1	7.19	123.90	120.30
1	H	29	GLU	C-N-CD	6.85	142.78	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	120	LEU	N-CA-C	5.86	126.83	111.00
3	J	120	LEU	N-CA-C	5.66	126.28	111.00
1	H	28	LEU	CA-CB-CG	5.61	128.21	115.30
1	H	28	LEU	CB-CG-CD2	5.18	119.81	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	120	LEU	Peptide
3	J	120	LEU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2328	0	2380	63	0
1	B	1667	0	1692	58	0
1	G	1730	0	1756	68	0
1	H	1662	0	1687	57	0
2	C	10570	0	10582	262	0
2	I	10566	0	10576	270	0
3	D	9107	0	9307	273	0
3	J	10369	0	10588	304	0
4	E	691	0	695	16	0
4	K	627	0	634	14	0
5	F	4204	0	4106	94	0
5	L	4196	0	4103	102	0
6	C	20	0	11	8	0
6	I	20	0	11	8	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0
8	D	2	0	0	0	0
8	J	2	0	0	0	0
All	All	57763	0	58128	1413	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1413) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.47	0.97
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.50	0.93
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.50	0.92
3:D:418:GLU:HG3	4:E:45:LYS:H	1.34	0.92
2:C:555:TYR:HD2	6:C:2001:4OB:H9	1.37	0.90
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.50	0.89
3:J:133:ARG:HB2	5:L:88:GLU:HA	1.58	0.85
2:I:555:TYR:HD2	6:I:2001:4OB:H9	1.42	0.84
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.60	0.83
3:J:1044:GLN:HB3	3:J:1071:GLY:HA3	1.59	0.83
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.61	0.83
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.62	0.82
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.28	0.81
1:B:191:ARG:HH22	3:D:409:TRP:HB3	1.45	0.81
2:C:1312:ASN:HD21	2:C:1314:GLN:HE21	1.28	0.81
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.64	0.80
3:J:905:ARG:HH11	4:K:16:ARG:HD2	1.47	0.80
2:C:1065:LYS:HE2	3:D:463:GLY:HA3	1.60	0.80
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.64	0.79
3:D:392:THR:HG21	5:F:606:VAL:HA	1.65	0.78
2:I:1065:LYS:HE2	3:J:463:GLY:HA3	1.63	0.78
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.66	0.78
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.64	0.78
2:I:806:PRO:HA	2:I:811:ASN:HD21	1.49	0.78
3:D:120:LEU:HD22	3:D:121:PRO:HD3	1.67	0.77
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.66	0.77
1:G:99:ILE:HG12	1:G:145:LYS:HG2	1.66	0.77
2:C:953:LEU:HD11	2:C:1033:ARG:HG3	1.66	0.77
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.68	0.76
2:I:873:ILE:HG13	2:I:944:ARG:HH22	1.50	0.76
1:A:99:ILE:HG12	1:A:145:LYS:HG2	1.67	0.76
2:I:953:LEU:HD11	2:I:1033:ARG:HG3	1.66	0.76
1:G:12:ARG:HG3	1:H:230:ALA:HB1	1.67	0.75
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.52	0.75
1:B:101:THR:HG22	1:B:116:THR:HB	1.68	0.75
2:I:215:TYR:HA	2:I:219:GLN:NE2	2.02	0.75
5:F:479:THR:HG22	5:F:482:GLU:HB2	1.69	0.74
3:J:418:GLU:HG3	4:K:45:LYS:H	1.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:133:ARG:NH2	5:F:93:ARG:O	2.19	0.74
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.67	0.74
1:H:101:THR:HG22	1:H:116:THR:HB	1.68	0.74
5:L:479:THR:HG22	5:L:482:GLU:HB2	1.69	0.74
1:G:225:ALA:HA	1:G:228:LEU:HD23	1.70	0.74
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.69	0.74
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.51	0.74
1:A:45:ARG:NH2	2:C:1215:GLY:O	2.21	0.73
2:I:840:SER:HB2	2:I:850:ILE:HD11	1.69	0.73
3:D:514:THR:HG23	3:D:576:ARG:HG2	1.71	0.72
2:I:452:ARG:NH1	2:I:584:TYR:O	2.22	0.72
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.23	0.72
2:I:292:ILE:HB	2:I:322:LEU:HD11	1.72	0.72
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.72	0.72
2:I:10:ARG:NH2	2:I:790:ASP:OD2	2.23	0.72
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.72	0.72
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.69	0.71
5:L:561:MET:HA	5:L:567:MET:HE1	1.71	0.71
3:D:905:ARG:HH11	4:E:16:ARG:HD2	1.54	0.71
3:J:514:THR:HG23	3:J:576:ARG:HG2	1.72	0.71
2:I:1106:ARG:HE	3:J:731:ARG:HH21	1.39	0.71
2:I:555:TYR:CD2	6:I:2001:4OB:H9	2.25	0.71
5:L:470:MET:HA	5:L:473:GLU:HB3	1.72	0.71
2:I:197:ARG:NH2	5:L:29:ASP:OD2	2.24	0.70
1:A:23:HIS:HB2	1:A:205:MET:O	1.91	0.70
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.55	0.70
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.54	0.70
3:J:342:LEU:HD11	3:J:1324:SER:HB3	1.72	0.70
1:G:23:HIS:HB2	1:G:205:MET:O	1.91	0.70
3:J:1026:PRO:HB2	3:J:1028:ILE:HG23	1.74	0.70
5:F:470:MET:HA	5:F:473:GLU:HB3	1.72	0.70
2:C:657:THR:HG21	2:C:1188:ASP:HB2	1.73	0.70
2:C:528:ARG:NH2	2:C:576:SER:O	2.25	0.70
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.72	0.70
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.72	0.70
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.73	0.70
3:J:1035:VAL:HG21	3:J:1121:LEU:HD21	1.74	0.70
2:C:555:TYR:CD2	6:C:2001:4OB:H9	2.25	0.69
5:F:561:MET:HA	5:F:567:MET:HE1	1.73	0.69
2:C:1106:ARG:HE	3:D:731:ARG:HH21	1.40	0.69
2:C:452:ARG:NH1	2:C:584:TYR:O	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:155:GLU:HB2	3:D:158:GLN:HB2	1.74	0.69
2:I:528:ARG:NH2	2:I:576:SER:O	2.25	0.69
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.74	0.69
5:F:134:VAL:HG21	5:F:266:PHE:HE1	1.58	0.68
2:C:292:ILE:HB	2:C:322:LEU:HD11	1.74	0.68
1:H:59:VAL:O	1:H:171:LEU:N	2.27	0.68
3:J:806:ASP:HA	3:J:1347:LEU:HD13	1.76	0.68
5:L:134:VAL:HG21	5:L:266:PHE:HE1	1.59	0.68
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.76	0.68
2:C:732:ILE:HG21	2:C:783:LEU:HD12	1.76	0.68
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.76	0.67
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.74	0.67
3:D:806:ASP:HA	3:D:1347:LEU:HD13	1.76	0.67
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.77	0.67
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.76	0.67
1:H:29:GLU:HB3	1:H:30:PRO:HD3	1.77	0.66
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.75	0.66
3:J:532:GLU:HA	3:J:535:ARG:HB3	1.76	0.66
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.78	0.66
5:F:602:SER:H	5:F:605:GLU:CG	2.08	0.66
2:I:463:GLN:HG3	2:I:505:PHE:HB2	1.78	0.66
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.76	0.66
3:J:749:LYS:HD3	3:J:753:SER:O	1.95	0.66
2:I:88:ARG:NH2	2:I:1035:LYS:O	2.28	0.66
3:D:749:LYS:HD3	3:D:753:SER:O	1.96	0.66
3:D:1310:THR:HG21	5:F:70:ASN:HA	1.76	0.66
1:H:33:ARG:HH11	2:I:1081:PRO:HG3	1.61	0.66
3:D:342:LEU:HD11	3:D:1324:SER:HB3	1.75	0.66
2:I:829:THR:HA	2:I:1059:ARG:HA	1.78	0.65
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.77	0.65
3:J:664:ILE:HG22	3:J:678:ARG:HG2	1.77	0.65
2:C:18:ARG:NH2	2:C:620:ASN:OD1	2.30	0.65
2:C:734:ILE:HD11	2:C:783:LEU:HD11	1.77	0.65
1:G:166:ARG:O	1:G:168:ILE:N	2.30	0.65
2:I:18:ARG:NH2	2:I:620:ASN:OD1	2.28	0.65
2:C:829:THR:HA	2:C:1059:ARG:HA	1.78	0.65
2:C:1320:PRO:HG2	3:D:1354:GLY:HA3	1.78	0.65
2:C:18:ARG:NH1	2:C:621:SER:O	2.30	0.64
2:I:13:LYS:HZ3	2:I:1151:LEU:HD12	1.61	0.64
1:A:166:ARG:O	1:A:168:ILE:N	2.30	0.64
2:I:976:ARG:HD2	2:I:989:LEU:HD23	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:664:ILE:HG22	3:D:678:ARG:HG2	1.79	0.64
1:B:133:LEU:HD11	1:B:140:ILE:HG21	1.79	0.64
3:D:532:GLU:HA	3:D:535:ARG:HB3	1.79	0.64
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.80	0.64
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	1.81	0.63
3:J:646:ILE:HD11	3:J:764:ARG:HD2	1.79	0.63
2:I:18:ARG:NH1	2:I:621:SER:O	2.31	0.63
1:A:61:ILE:HG22	1:A:62:ASP:H	1.64	0.63
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.13	0.63
5:L:593:LYS:HE2	5:L:596:ARG:HD3	1.81	0.63
3:D:356:THR:OG1	3:D:357:VAL:N	2.32	0.63
3:D:646:ILE:HD11	3:D:764:ARG:HD2	1.80	0.63
5:F:602:SER:H	5:F:605:GLU:CD	2.02	0.63
5:F:561:MET:HG2	5:F:576:VAL:HG22	1.81	0.63
1:B:13:LEU:HD12	1:B:29:GLU:HB2	1.79	0.63
3:D:682:VAL:O	3:D:685:ILE:HG12	1.99	0.63
3:J:262:THR:OG1	3:J:266:ASN:ND2	2.32	0.63
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.81	0.62
2:C:1238:LEU:HD12	2:C:1238:LEU:H	1.64	0.62
2:C:814:ASP:OD2	2:C:1106:ARG:NH1	2.29	0.62
2:C:976:ARG:HD2	2:C:989:LEU:HD23	1.80	0.62
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.81	0.62
2:I:213:LEU:HB3	2:I:422:LYS:HD2	1.79	0.62
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.32	0.62
1:G:39:LEU:HD11	1:H:227:GLN:HB3	1.81	0.62
1:G:61:ILE:HG22	1:G:62:ASP:H	1.63	0.62
1:H:133:LEU:HD11	1:H:140:ILE:HG21	1.79	0.62
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.81	0.62
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.82	0.62
1:B:100:LEU:HD21	1:B:121:VAL:HG11	1.81	0.62
3:D:1174:ARG:HG2	3:D:1189:MET:HG2	1.81	0.62
2:C:103:VAL:HG12	2:C:116:ASP:HB3	1.82	0.62
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.82	0.62
3:J:325:LYS:HD3	5:L:508:GLU:HG2	1.80	0.61
3:D:308:ASP:OD2	3:D:311:ARG:NH2	2.32	0.61
1:A:70:THR:HG21	2:C:755:LYS:HE2	1.82	0.61
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.66	0.61
1:A:31:LEU:HD11	1:A:201:LEU:HB2	1.83	0.61
2:C:136:PHE:O	2:C:143:ARG:N	2.28	0.61
2:I:1157:GLN:HG3	2:I:1159:VAL:HG13	1.81	0.61
1:G:45:ARG:HH22	2:I:1216:ARG:HA	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1101:LEU:HD21	3:J:508:LEU:HD22	1.82	0.61
3:J:1174:ARG:HG2	3:J:1189:MET:HG2	1.82	0.61
2:I:149:LEU:HD13	2:I:453:ILE:HG13	1.82	0.61
1:B:73:GLY:HA2	1:B:134:THR:HG22	1.83	0.60
2:C:1157:GLN:HG3	2:C:1159:VAL:HG13	1.81	0.60
1:G:14:VAL:HG22	1:G:15:ASP:H	1.64	0.60
3:J:1172:LYS:HA	3:J:1191:PRO:HA	1.83	0.60
3:J:741:ALA:O	3:J:762:ASN:ND2	2.33	0.60
1:B:62:ASP:OD2	1:B:71:LYS:NZ	2.35	0.60
3:D:133:ARG:HB2	5:F:88:GLU:HA	1.83	0.60
1:H:83:LEU:HA	1:H:86:LYS:HE2	1.83	0.60
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.83	0.60
2:C:120:GLN:HG3	2:C:121:GLU:HG2	1.82	0.60
3:D:1172:LYS:HA	3:D:1191:PRO:HA	1.83	0.60
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.82	0.60
3:D:741:ALA:O	3:D:762:ASN:ND2	2.34	0.60
1:B:33:ARG:HH11	2:C:1081:PRO:HG3	1.66	0.60
3:D:1238:GLN:NE2	3:D:1248:ILE:O	2.35	0.60
3:D:341:ASN:HB2	3:D:1352:ILE:HD13	1.83	0.60
1:H:191:ARG:NH2	3:J:410:ASP:OD2	2.35	0.60
1:A:14:VAL:HG22	1:A:15:ASP:H	1.67	0.60
2:C:746:ALA:HA	2:C:974:ARG:HH21	1.66	0.60
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.67	0.60
3:J:527:LEU:HD23	3:J:532:GLU:HG3	1.84	0.60
5:L:561:MET:HG2	5:L:576:VAL:HG22	1.84	0.60
2:C:1287:LEU:HD13	3:D:1357:ILE:HD11	1.84	0.60
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.34	0.59
3:J:308:ASP:OD2	3:J:311:ARG:NH2	2.34	0.59
1:B:83:LEU:HA	1:B:86:LYS:HE2	1.84	0.59
2:C:841:ARG:HA	2:C:1046:VAL:HA	1.84	0.59
6:C:2001:4OB:H8	3:D:773:PHE:HB3	1.82	0.59
3:D:304:ASP:OD2	3:D:312:ARG:NH2	2.34	0.59
3:J:1050:THR:HG23	3:J:1057:SER:HB3	1.84	0.59
3:J:1157:ALA:HB2	3:J:1210:ILE:HD11	1.84	0.59
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.83	0.59
3:J:425:ARG:HD2	3:J:459:ALA:HB2	1.84	0.59
5:L:305:LEU:HD13	5:L:315:TRP:HA	1.84	0.59
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.85	0.59
2:I:269:ILE:HG23	2:I:273:HIS:HB2	1.85	0.59
3:J:682:VAL:O	3:J:685:ILE:HG12	2.02	0.59
4:K:15:ASN:HB3	4:K:18:ASP:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:476:ARG:HG2	5:L:477:GLU:HG2	1.84	0.59
4:E:15:ASN:HB3	4:E:18:ASP:HB2	1.84	0.59
4:E:73:GLN:HA	4:E:76:GLU:HB2	1.85	0.59
5:F:292:VAL:HG21	5:F:299:LYS:HG3	1.83	0.59
2:I:40:GLU:O	2:I:73:TYR:OH	2.20	0.59
3:J:356:THR:OG1	3:J:357:VAL:N	2.36	0.59
5:L:551:LEU:HD22	5:L:597:LYS:HD2	1.85	0.59
3:D:847:ASP:OD1	3:D:847:ASP:N	2.35	0.59
1:G:25:LYS:HG2	1:G:204:GLU:HG3	1.84	0.59
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.84	0.59
1:G:45:ARG:NH2	2:I:1215:GLY:O	2.33	0.59
2:I:1106:ARG:HD2	2:I:1106:ARG:H	1.67	0.59
2:I:841:ARG:HA	2:I:1046:VAL:HA	1.84	0.59
3:J:892:PHE:H	3:J:1281:GLU:HG2	1.68	0.59
5:L:292:VAL:HG21	5:L:299:LYS:HG3	1.84	0.59
3:J:1238:GLN:NE2	3:J:1248:ILE:O	2.35	0.59
6:I:2001:4OB:H8	3:J:773:PHE:HB3	1.84	0.59
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.84	0.59
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.85	0.58
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.85	0.58
3:D:194:LEU:HD13	3:D:228:VAL:HG22	1.85	0.58
3:J:304:ASP:OD2	3:J:312:ARG:NH2	2.36	0.58
5:F:551:LEU:HD22	5:F:597:LYS:HD2	1.84	0.58
2:I:494:ASN:OD1	2:I:495:ALA:N	2.34	0.58
5:F:305:LEU:HD13	5:F:315:TRP:HA	1.84	0.58
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.67	0.58
2:C:339:ASN:HB3	2:C:343:HIS:H	1.69	0.58
3:D:650:LYS:HE2	3:D:654:ILE:HD11	1.85	0.58
2:C:897:PRO:HG3	3:D:77:ARG:HH22	1.67	0.58
5:F:461:ASN:O	5:F:465:ARG:HG2	2.04	0.58
1:A:25:LYS:HG2	1:A:204:GLU:HG3	1.85	0.58
1:G:10:LYS:HE2	1:H:229:GLU:HB3	1.84	0.58
3:J:34:SER:OG	3:J:104:HIS:ND1	2.26	0.58
3:J:152:THR:OG1	3:J:153:ASN:N	2.36	0.58
2:C:102:LEU:HB2	2:C:489:PRO:HG3	1.86	0.58
3:D:363:LEU:HD23	3:D:487:THR:HG22	1.86	0.58
1:G:31:LEU:HD11	1:G:201:LEU:HB2	1.84	0.58
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.86	0.58
2:C:40:GLU:O	2:C:73:TYR:OH	2.20	0.58
2:I:272:ARG:HA	2:I:275:ARG:HD2	1.86	0.58
5:F:276:MET:SD	5:F:279:ARG:NH1	2.77	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:398:LYS:HE2	5:F:532:LEU:HD23	1.86	0.58
1:H:73:GLY:HA2	1:H:134:THR:HG22	1.84	0.58
1:A:282:VAL:HB	1:A:316:MET:HB2	1.86	0.57
1:H:62:ASP:OD2	1:H:71:LYS:NZ	2.37	0.57
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.68	0.57
2:C:897:PRO:HB3	5:F:564:GLY:C	2.25	0.57
1:G:29:GLU:HB3	1:G:30:PRO:HD3	1.86	0.57
3:J:847:ASP:N	3:J:847:ASP:OD1	2.33	0.57
2:C:494:ASN:OD1	2:C:495:ALA:N	2.34	0.57
5:F:278:ASP:OD1	5:F:281:ARG:NH1	2.37	0.57
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.85	0.57
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.37	0.57
3:J:194:LEU:HD13	3:J:228:VAL:HG22	1.87	0.57
2:I:1185:PRO:HD2	2:I:1189:GLY:HA2	1.87	0.57
5:F:476:ARG:HG2	5:F:477:GLU:HG2	1.87	0.57
2:C:1142:ARG:HH22	2:C:1165:SER:HB2	1.69	0.57
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.40	0.57
3:D:1227:HIS:HA	3:D:1230:THR:HG22	1.86	0.57
2:I:94:ALA:HB2	2:I:129:LEU:HD11	1.86	0.57
5:L:225:ARG:O	5:L:229:VAL:HG13	2.04	0.57
3:D:892:PHE:H	3:D:1281:GLU:HG2	1.69	0.57
1:H:182:ARG:NH1	3:J:581:MET:SD	2.78	0.57
2:I:207:THR:HG21	2:I:351:LEU:HG	1.86	0.57
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.19	0.57
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.86	0.57
3:D:388:ARG:NH1	3:D:414:GLU:OE1	2.38	0.57
5:F:49:ASN:HA	5:F:53:ILE:HA	1.87	0.57
2:C:518:ASN:OD1	2:C:518:ASN:N	2.36	0.56
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.86	0.56
1:H:59:VAL:HG21	1:H:85:LEU:HD13	1.85	0.56
5:F:515:GLU:HG2	5:F:516:ASP:H	1.70	0.56
2:I:814:ASP:OD2	2:I:1106:ARG:NH1	2.32	0.56
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.87	0.56
2:C:1119:MET:HE3	2:C:1204:LEU:HD13	1.87	0.56
2:C:1276:TRP:CZ2	3:D:801:VAL:HG21	2.40	0.56
2:I:102:LEU:HB2	2:I:489:PRO:HG3	1.87	0.56
3:J:210:SER:O	3:J:214:ARG:HG2	2.05	0.56
1:A:60:GLU:HB2	1:A:170:ARG:HG2	1.88	0.56
3:D:148:GLU:H	3:D:156:ARG:HG3	1.70	0.56
3:D:527:LEU:HD23	3:D:532:GLU:HG3	1.86	0.56
2:I:1142:ARG:HH22	2:I:1165:SER:HB2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:518:ASN:N	2:I:518:ASN:OD1	2.37	0.56
3:D:854:ALA:HB2	3:J:1372:ARG:HB2	1.88	0.56
3:J:960:LEU:HB3	3:J:963:VAL:HG11	1.86	0.56
1:B:59:VAL:HG21	1:B:85:LEU:HD13	1.87	0.56
1:H:32:GLU:OE1	1:H:195:ARG:NH2	2.39	0.56
3:J:1273:ASP:OD1	3:J:1274:PHE:N	2.38	0.56
3:J:148:GLU:H	3:J:156:ARG:HG3	1.69	0.56
6:I:2001:4OB:H7	3:J:774:ILE:CG1	2.35	0.56
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.87	0.56
2:I:560:PRO:O	3:J:780:ARG:NH2	2.30	0.56
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.39	0.56
5:L:278:ASP:OD1	5:L:281:ARG:NH1	2.38	0.56
5:L:49:ASN:HA	5:L:53:ILE:HA	1.87	0.56
1:A:155:ALA:HA	1:A:158:ARG:HG3	1.88	0.56
1:B:29:GLU:HA	1:B:200:LYS:HG3	1.86	0.56
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.38	0.56
3:D:115:TRP:O	3:D:119:SER:HB2	2.06	0.56
3:D:1181:ASP:HA	3:J:202:ARG:HD3	1.88	0.56
1:B:32:GLU:OE1	1:B:195:ARG:NH2	2.39	0.56
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.86	0.56
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.88	0.56
3:D:817:HIS:CE1	3:D:860:ARG:HE	2.23	0.56
2:I:30:ILE:H	2:I:30:ILE:HD12	1.70	0.56
5:L:515:GLU:HG2	5:L:516:ASP:H	1.70	0.56
5:L:602:SER:H	5:L:605:GLU:HG3	1.71	0.56
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.88	0.56
1:G:44:ARG:HG3	1:G:183:ILE:HG22	1.87	0.56
2:C:138:ILE:HB	2:C:143:ARG:HD3	1.88	0.56
3:D:1273:ASP:OD1	3:D:1274:PHE:N	2.38	0.56
4:E:39:VAL:HG22	4:E:40:PRO:HD2	1.88	0.56
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.71	0.55
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.89	0.55
2:I:1151:LEU:HD21	2:I:1198:LEU:HD23	1.87	0.55
2:I:176:ILE:HD12	2:I:184:LEU:HD23	1.88	0.55
1:A:29:GLU:HB3	1:A:30:PRO:HD3	1.87	0.55
1:B:98:VAL:HG11	1:B:121:VAL:HG22	1.87	0.55
2:C:1151:LEU:HD21	2:C:1198:LEU:HD23	1.87	0.55
3:D:210:SER:O	3:D:214:ARG:HG2	2.07	0.55
3:J:114:ILE:HD12	3:J:304:ASP:HB3	1.87	0.55
1:A:44:ARG:HG3	1:A:183:ILE:HG22	1.88	0.55
2:C:149:LEU:HD13	2:C:453:ILE:HG13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:152:THR:OG1	3:D:153:ASN:N	2.38	0.55
1:G:60:GLU:HB2	1:G:170:ARG:HG2	1.87	0.55
2:I:1119:MET:HE3	2:I:1204:LEU:HD13	1.89	0.55
3:J:120:LEU:HD22	3:J:121:PRO:HD3	1.88	0.55
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.88	0.55
2:C:1101:LEU:HD21	3:D:508:LEU:HD22	1.88	0.55
2:C:207:THR:HG21	2:C:351:LEU:HG	1.89	0.55
3:D:474:LEU:HD23	4:E:28:ARG:HG2	1.88	0.55
3:J:1350:ASN:HA	3:J:1353:VAL:HG12	1.89	0.55
3:J:79:LYS:HB2	5:L:569:THR:H	1.70	0.55
1:H:91:ARG:HG3	1:H:122:GLU:HB3	1.89	0.55
3:J:141:PHE:HD1	3:J:180:MET:HG3	1.69	0.55
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.89	0.55
2:I:215:TYR:HA	2:I:219:GLN:HE21	1.72	0.55
3:D:1293:GLU:H	3:J:1226:VAL:HB	1.71	0.55
1:G:11:PRO:HD2	1:H:227:GLN:HA	1.89	0.55
2:I:1320:PRO:HG2	3:J:1354:GLY:HA3	1.88	0.55
3:J:388:ARG:NH1	3:J:414:GLU:OE1	2.39	0.55
5:L:244:THR:O	5:L:247:GLU:HG2	2.06	0.55
2:I:197:ARG:HH12	5:L:29:ASP:HB3	1.71	0.55
3:J:79:LYS:HB2	5:L:569:THR:N	2.22	0.55
2:C:30:ILE:H	2:C:30:ILE:HD12	1.70	0.54
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.88	0.54
1:H:98:VAL:HG11	1:H:121:VAL:HG22	1.89	0.54
2:I:302:ILE:HG22	2:I:309:LEU:HA	1.89	0.54
2:I:6:THR:HG21	2:I:782:VAL:HG23	1.89	0.54
3:J:115:TRP:O	3:J:119:SER:HB2	2.06	0.54
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.55	0.54
5:L:290:LEU:HB3	5:L:333:VAL:HG21	1.89	0.54
1:B:51:MET:HB3	1:B:178:SER:HA	1.89	0.54
2:C:9:LYS:HA	2:C:1171:ARG:HD2	1.89	0.54
3:J:757:THR:OG1	3:J:757:THR:O	2.25	0.54
1:B:37:HIS:CE1	2:C:1216:ARG:HD2	2.43	0.54
3:J:817:HIS:CE1	3:J:860:ARG:HE	2.24	0.54
2:C:363:LEU:HB3	2:C:381:ALA:HB1	1.89	0.54
2:I:668:ILE:HD11	2:I:683:ALA:HB2	1.89	0.54
1:A:50:SER:HB3	1:A:150:ARG:HD2	1.88	0.54
5:F:111:LEU:HD13	5:F:116:GLU:HG2	1.90	0.54
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.88	0.54
3:D:114:ILE:HD12	3:D:304:ASP:HB3	1.89	0.54
3:D:73:GLY:O	3:D:76:LYS:NZ	2.31	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:872:LEU:HD22	3:D:877:VAL:HG11	1.90	0.54
1:G:155:ALA:HA	1:G:158:ARG:HG3	1.89	0.54
3:J:733:SER:O	3:J:737:ILE:HG12	2.08	0.54
5:L:276:MET:SD	5:L:279:ARG:NH1	2.80	0.54
3:D:798:ARG:NH1	3:D:802:ASP:OD2	2.41	0.54
2:I:820:GLU:HA	2:I:1079:ILE:HD11	1.90	0.54
3:J:613:GLY:O	3:J:617:THR:OG1	2.26	0.54
5:L:111:LEU:HD13	5:L:116:GLU:HG2	1.90	0.54
5:L:551:LEU:HD11	5:L:598:LEU:HD21	1.88	0.54
1:G:31:LEU:HD13	1:G:36:GLY:HA2	1.90	0.54
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.90	0.54
2:I:9:LYS:HA	2:I:1171:ARG:HD2	1.89	0.54
3:D:757:THR:OG1	3:D:757:THR:O	2.25	0.54
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.90	0.53
2:I:1287:LEU:HD13	3:J:1357:ILE:HD11	1.89	0.53
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.90	0.53
2:C:555:TYR:HA	3:D:773:PHE:HE1	1.72	0.53
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.73	0.53
5:F:479:THR:HG23	5:F:481:GLU:H	1.73	0.53
1:H:23:HIS:ND1	1:H:206:GLU:HG2	2.23	0.53
2:I:61:SER:HB3	2:I:479:LEU:HB3	1.90	0.53
2:I:808:ASN:H	3:J:633:ALA:HB2	1.73	0.53
5:L:479:THR:HG23	5:L:481:GLU:H	1.73	0.53
3:D:683:ILE:HD11	3:D:754:ILE:HG23	1.90	0.53
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.90	0.53
2:I:1275:VAL:HG13	2:I:1287:LEU:HD11	1.88	0.53
2:I:124:MET:HB2	2:I:498:ILE:HD13	1.89	0.53
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.91	0.53
2:I:237:LEU:HD22	2:I:237:LEU:H	1.73	0.53
3:J:749:LYS:HB2	3:J:750:PRO:CD	2.38	0.53
3:J:798:ARG:NH1	3:J:802:ASP:OD2	2.42	0.53
5:L:448:ARG:NH1	5:L:501:ALA:O	2.34	0.53
2:C:870:ILE:HB	2:C:944:ARG:HD3	1.91	0.53
3:D:34:SER:OG	3:D:104:HIS:ND1	2.30	0.53
2:I:590:PRO:HG3	2:I:605:TYR:CZ	2.42	0.53
1:A:153:VAL:HB	1:A:175:ALA:HB3	1.91	0.53
1:A:31:LEU:HD13	1:A:36:GLY:HA2	1.90	0.53
3:D:77:ARG:HG3	3:D:79:LYS:H	1.74	0.53
3:J:363:LEU:HD23	3:J:487:THR:HG22	1.91	0.53
2:I:1276:TRP:CZ2	3:J:801:VAL:HG21	2.43	0.53
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:506:VAL:HG23	3:J:628:GLY:HA3	1.91	0.53
3:D:478:LEU:HG	4:E:47:THR:HG23	1.89	0.53
3:D:609:TYR:HB2	3:D:617:THR:HG21	1.89	0.53
1:G:153:VAL:HB	1:G:175:ALA:HB3	1.91	0.53
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.44	0.53
2:C:668:ILE:HD11	2:C:683:ALA:HB2	1.90	0.53
6:I:2001:4OB:H5	3:J:755:ILE:HG12	1.74	0.53
2:C:13:LYS:HZ3	2:C:1151:LEU:HD12	1.73	0.52
3:D:1350:ASN:HA	3:D:1353:VAL:HG12	1.90	0.52
3:J:1227:HIS:HA	3:J:1230:THR:HG22	1.91	0.52
3:J:73:GLY:O	3:J:76:LYS:NZ	2.33	0.52
1:B:23:HIS:ND1	1:B:206:GLU:HG2	2.24	0.52
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.09	0.52
5:F:165:PHE:CE2	5:F:217:ALA:HA	2.44	0.52
3:J:958:ILE:HD11	3:J:1017:VAL:HG11	1.91	0.52
3:J:279:LEU:HD11	3:J:296:LYS:HG2	1.92	0.52
3:D:749:LYS:HB2	3:D:750:PRO:CD	2.39	0.52
5:F:482:GLU:O	5:F:486:ARG:NH2	2.42	0.52
2:C:103:VAL:HB	2:C:113:THR:HG21	1.90	0.52
3:D:613:GLY:O	3:D:617:THR:OG1	2.27	0.52
2:C:734:ILE:HD12	2:C:777:VAL:HG21	1.92	0.52
3:D:28:ASP:OD1	3:D:31:ARG:NH1	2.43	0.52
3:D:585:LYS:HB2	3:D:612:LEU:HD21	1.91	0.52
2:I:718:ALA:HB2	2:I:783:LEU:HD23	1.92	0.52
2:C:95:PRO:HA	2:C:126:GLU:HG2	1.91	0.52
2:I:1282:GLY:O	3:J:1361:THR:OG1	2.23	0.52
5:L:165:PHE:CE2	5:L:217:ALA:HA	2.44	0.52
1:A:285:THR:HG23	1:A:288:GLU:H	1.75	0.52
1:A:93:GLN:H	1:A:120:ASP:HB3	1.75	0.52
1:B:64:VAL:HG21	1:B:69:SER:HB3	1.91	0.52
3:D:279:LEU:HD11	3:D:296:LYS:HG2	1.91	0.52
5:F:397:ARG:HG2	5:F:443:ILE:HG21	1.92	0.52
1:H:64:VAL:HG21	1:H:69:SER:HB3	1.91	0.52
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.10	0.52
1:A:26:VAL:HG22	1:A:203:ILE:HB	1.92	0.52
1:A:91:ARG:HD3	1:A:210:THR:O	2.10	0.52
1:A:225:ALA:HA	1:A:228:LEU:HD23	1.92	0.52
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.75	0.52
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.45	0.52
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.09	0.52
3:D:325:LYS:HD3	5:F:508:GLU:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1246:ARG:NE	3:J:348:ASP:OD1	2.42	0.52
3:J:609:TYR:HB2	3:J:617:THR:HG21	1.92	0.52
3:J:263:SER:HB2	5:L:507:MET:HE2	1.91	0.52
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.91	0.52
2:C:1176:LEU:HD13	2:C:1180:MET:HG2	1.91	0.52
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.92	0.52
5:L:483:LEU:H	5:L:483:LEU:HD12	1.74	0.52
2:I:1149:TYR:HB3	2:I:1159:VAL:HG11	1.91	0.51
2:I:349:GLU:O	2:I:353:VAL:HG23	2.10	0.51
2:C:615:VAL:HG13	2:C:650:VAL:HA	1.92	0.51
2:C:6:THR:HG21	2:C:782:VAL:HG23	1.90	0.51
1:G:231:PHE:CE1	1:H:28:LEU:HD11	2.45	0.51
2:I:739:ASP:N	2:I:739:ASP:OD1	2.37	0.51
3:J:28:ASP:OD1	3:J:31:ARG:NH1	2.43	0.51
3:J:425:ARG:HG2	3:J:426:ALA:H	1.75	0.51
2:C:903:ARG:O	2:C:907:GLY:N	2.43	0.51
1:G:118:ASP:HB3	1:G:121:VAL:HG23	1.92	0.51
2:I:227:LYS:O	2:I:245:ARG:NH2	2.43	0.51
2:C:488:MET:O	2:C:490:GLN:N	2.37	0.51
1:G:12:ARG:H	1:G:30:PRO:HD2	1.75	0.51
1:H:48:LEU:HD12	1:H:183:ILE:HD11	1.93	0.51
1:H:91:ARG:HG2	1:H:122:GLU:O	2.11	0.51
2:C:817:LEU:HD11	2:C:1080:ASN:HD22	1.75	0.51
1:G:231:PHE:HE1	1:H:28:LEU:HD11	1.74	0.51
3:J:189:LEU:HD22	3:J:234:PRO:HB3	1.91	0.51
3:D:425:ARG:HG2	3:D:426:ALA:H	1.75	0.51
5:F:402:LEU:HA	5:F:405:ILE:HG12	1.93	0.51
5:F:489:MET:HB2	5:F:490:PRO:HD2	1.93	0.51
1:G:11:PRO:HA	1:G:30:PRO:HB2	1.93	0.51
2:I:149:LEU:HB2	2:I:530:ILE:HG22	1.91	0.51
1:G:70:THR:HG21	2:I:755:LYS:HE2	1.93	0.51
3:J:478:LEU:HG	4:K:47:THR:HG23	1.91	0.51
2:C:820:GLU:HA	2:C:1079:ILE:HD11	1.92	0.51
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.92	0.51
2:C:176:ILE:HD12	2:C:184:LEU:HD23	1.92	0.51
2:C:42:ASP:C	2:C:44:GLU:H	2.14	0.51
3:D:733:SER:O	3:D:737:ILE:HG12	2.10	0.51
2:I:734:ILE:HD12	2:I:777:VAL:HG21	1.92	0.51
2:I:757:THR:HG23	2:I:765:ILE:HG23	1.91	0.51
5:L:482:GLU:O	5:L:486:ARG:NH2	2.44	0.51
5:F:483:LEU:H	5:F:483:LEU:HD12	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:615:VAL:HG13	2:I:650:VAL:HA	1.92	0.51
3:J:147:ILE:HG22	3:J:188:LEU:HG	1.93	0.51
6:C:2001:4OB:H5	3:D:755:ILE:HG12	1.75	0.51
3:D:77:ARG:HE	5:F:569:THR:HA	1.75	0.51
1:H:100:LEU:HD11	1:H:121:VAL:HG21	1.92	0.51
2:I:324:LYS:O	2:I:327:GLN:NE2	2.43	0.51
3:J:1267:VAL:HB	3:J:1301:THR:OG1	2.10	0.51
3:J:585:LYS:HB2	3:J:612:LEU:HD21	1.92	0.51
1:B:91:ARG:HG3	1:B:122:GLU:HB3	1.92	0.51
2:C:718:ALA:HB2	2:C:783:LEU:HD23	1.93	0.51
2:C:758:ARG:NH1	2:C:835:GLU:OE1	2.43	0.51
2:I:103:VAL:HB	2:I:113:THR:HG21	1.92	0.51
3:J:341:ASN:HB2	3:J:1352:ILE:HD13	1.93	0.51
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.92	0.50
2:I:97:ARG:HB3	2:I:121:GLU:HB2	1.93	0.50
2:I:136:PHE:CE2	2:I:456:VAL:HG11	2.45	0.50
2:I:819:SER:HB2	2:I:1085:MET:HG3	1.92	0.50
2:C:936:ARG:NH2	2:C:1043:ALA:O	2.44	0.50
2:C:227:LYS:O	2:C:245:ARG:NH2	2.45	0.50
2:C:560:PRO:CB	3:D:776:THR:HG21	2.42	0.50
5:F:441:ARG:NH1	5:F:445:ASP:OD1	2.45	0.50
5:L:397:ARG:HG2	5:L:443:ILE:HG21	1.92	0.50
2:C:672:GLU:HG2	2:C:1187:PHE:HA	1.93	0.50
3:D:682:VAL:HA	3:D:685:ILE:CD1	2.41	0.50
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.75	0.50
2:I:241:LEU:HD21	2:I:246:LEU:HD11	1.94	0.50
2:I:488:MET:O	2:I:490:GLN:N	2.39	0.50
3:J:750:PRO:HA	3:J:777:HIS:CE1	2.47	0.50
3:J:752:GLY:O	3:J:754:ILE:N	2.45	0.50
5:L:489:MET:HB2	5:L:490:PRO:HD2	1.93	0.50
3:J:77:ARG:HE	5:L:569:THR:HA	1.76	0.50
2:C:324:LYS:O	2:C:327:GLN:NE2	2.44	0.50
2:I:968:GLU:HG3	2:I:1018:TYR:HE1	1.76	0.50
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.12	0.50
3:D:1227:HIS:CG	3:J:1293:GLU:HG2	2.47	0.50
5:L:511:ILE:HG13	5:L:512:GLY:H	1.76	0.50
1:A:118:ASP:HB3	1:A:121:VAL:HG23	1.92	0.50
2:C:685:MET:SD	2:C:1073:LYS:HG2	2.51	0.50
1:G:182:ARG:O	1:G:206:GLU:N	2.44	0.50
1:G:26:VAL:HG22	1:G:203:ILE:HB	1.93	0.50
2:I:21:VAL:HG11	2:I:592:ARG:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:HG2	1:B:38:THR:HB	1.93	0.50
3:D:189:LEU:HD22	3:D:234:PRO:HB3	1.92	0.50
1:G:93:GLN:H	1:G:120:ASP:HB3	1.76	0.50
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.77	0.50
2:I:517:GLN:O	2:I:517:GLN:HG2	2.12	0.50
3:J:1162:ILE:HG23	3:J:1178:THR:HB	1.94	0.50
5:L:119:ILE:HA	5:L:122:ARG:HD3	1.94	0.50
3:D:824:PRO:HD3	3:D:835:LEU:HB2	1.94	0.50
1:B:100:LEU:HD11	1:B:121:VAL:HG21	1.93	0.50
2:C:896:THR:HB	2:C:897:PRO:HD2	1.93	0.50
5:F:119:ILE:HA	5:F:122:ARG:HD3	1.93	0.50
5:F:511:ILE:HG13	5:F:512:GLY:H	1.77	0.50
1:H:64:VAL:HG12	1:H:65:LEU:H	1.77	0.50
2:I:213:LEU:HD13	2:I:422:LYS:HG2	1.93	0.50
3:J:683:ILE:HD11	3:J:754:ILE:HG23	1.94	0.50
2:C:26:TYR:CZ	2:C:28:LEU:HB2	2.47	0.49
2:C:538:LEU:HD22	2:C:543:ALA:HB2	1.94	0.49
3:D:789:LYS:HA	3:D:792:ASN:HB2	1.93	0.49
2:I:692:THR:OG1	2:I:693:LEU:N	2.45	0.49
5:L:164:GLY:O	5:L:260:ARG:HB2	2.11	0.49
2:C:349:GLU:O	2:C:353:VAL:HG23	2.12	0.49
3:J:1343:GLU:HB3	3:J:1345:ARG:HD3	1.93	0.49
3:J:794:GLY:O	3:J:797:THR:OG1	2.26	0.49
1:B:91:ARG:HG2	1:B:122:GLU:O	2.12	0.49
3:J:368:LEU:HD22	3:J:373:ALA:HB2	1.94	0.49
1:A:45:ARG:HD3	2:C:1083:GLU:HB3	1.93	0.49
2:C:1149:TYR:HB3	2:C:1159:VAL:HG11	1.95	0.49
2:C:50:GLU:HG2	2:C:73:TYR:HE1	1.78	0.49
1:H:61:ILE:HB	1:H:64:VAL:O	2.12	0.49
2:I:657:THR:HG1	2:I:1187:PHE:HB2	1.77	0.49
2:I:387:ASN:HA	2:I:391:SER:HB2	1.94	0.49
3:J:1077:ALA:HB2	3:J:1100:PHE:CD1	2.47	0.49
3:J:1191:PRO:HB2	3:J:1194:ARG:HD3	1.93	0.49
3:J:124:ILE:HG23	3:J:189:LEU:HD11	1.95	0.49
1:B:64:VAL:HG12	1:B:65:LEU:H	1.78	0.49
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.47	0.49
2:C:968:GLU:HG3	2:C:1018:TYR:HE1	1.77	0.49
3:D:1135:THR:OG1	3:D:1136:GLY:N	2.46	0.49
2:I:545:PHE:CZ	3:J:781:LYS:HG3	2.47	0.49
3:J:1198:VAL:HG23	3:J:1204:VAL:HG11	1.94	0.49
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:250:THR:HA	2:C:268:ARG:HA	1.94	0.49
2:C:387:ASN:HA	2:C:391:SER:HB2	1.95	0.49
2:C:878:THR:OG1	2:C:879:GLY:N	2.45	0.49
3:D:1162:ILE:HG23	3:D:1178:THR:HB	1.94	0.49
2:I:685:MET:SD	2:I:1073:LYS:HG2	2.53	0.49
2:I:878:THR:OG1	2:I:879:GLY:N	2.45	0.49
3:J:268:LEU:HB3	3:J:306:LEU:HD23	1.94	0.49
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.77	0.49
2:C:124:MET:HB2	2:C:498:ILE:HD13	1.94	0.49
3:D:1341:ARG:HH22	3:D:1373:ARG:HH21	1.59	0.49
3:D:708:ASN:HB3	3:D:712:GLN:O	2.12	0.49
5:F:164:GLY:O	5:F:260:ARG:HB2	2.12	0.49
1:G:229:GLU:HG2	1:G:229:GLU:O	2.13	0.49
5:L:41:ILE:HA	5:L:44:ILE:HG23	1.94	0.49
2:C:1122:LYS:HG2	2:C:1229:TYR:CE1	2.47	0.49
6:C:2001:4OB:FAD	3:D:750:PRO:HD3	2.02	0.49
2:C:255:ILE:HB	2:C:263:VAL:HB	1.95	0.49
2:C:517:GLN:HG2	2:C:517:GLN:O	2.11	0.49
3:D:1286:LYS:O	3:D:1290:ARG:HB2	2.13	0.49
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.35	0.49
1:G:66:HIS:HA	1:G:171:LEU:HD11	1.95	0.49
2:I:672:GLU:HG2	2:I:1187:PHE:HA	1.95	0.49
1:A:182:ARG:O	1:A:206:GLU:N	2.45	0.49
2:C:149:LEU:HB2	2:C:530:ILE:HG22	1.95	0.49
3:D:298:MET:SD	5:F:402:LEU:HB3	2.53	0.49
2:I:26:TYR:CZ	2:I:28:LEU:HB2	2.47	0.49
5:L:548:LEU:HD21	5:L:559:LEU:HD23	1.95	0.49
3:D:268:LEU:HB3	3:D:306:LEU:HD23	1.94	0.49
1:G:50:SER:HB3	1:G:150:ARG:HD2	1.95	0.49
3:J:1024:THR:HG22	3:J:1026:PRO:HD3	1.93	0.49
6:I:2001:4OB:FAD	3:J:750:PRO:HD3	2.03	0.49
3:J:800:LEU:HB3	3:J:920:ALA:HB1	1.94	0.49
5:L:402:LEU:HA	5:L:405:ILE:HG12	1.94	0.49
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.78	0.48
2:C:242:VAL:HB	2:C:245:ARG:HD2	1.94	0.48
2:C:146:VAL:HG13	2:C:529:ARG:HB3	1.95	0.48
3:D:1280:VAL:HG11	3:D:1304:ARG:HH21	1.77	0.48
3:D:275:ARG:HD3	3:D:298:MET:HB3	1.95	0.48
1:G:91:ARG:HD3	1:G:210:THR:O	2.13	0.48
2:I:216:THR:O	2:I:219:GLN:HB2	2.13	0.48
3:J:1286:LYS:O	3:J:1290:ARG:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:ILE:HB	1:B:64:VAL:O	2.13	0.48
2:C:28:LEU:HD21	2:C:524:ILE:HG13	1.95	0.48
2:C:692:THR:OG1	2:C:693:LEU:N	2.45	0.48
5:F:281:ARG:O	5:F:285:ARG:HG3	2.13	0.48
1:H:54:CYS:SG	1:H:148:ARG:HG2	2.54	0.48
2:I:255:ILE:HB	2:I:263:VAL:HB	1.94	0.48
5:F:466:ILE:HD13	5:F:486:ARG:HB3	1.94	0.48
1:G:50:SER:HB3	1:H:8:PHE:HE1	1.76	0.48
3:J:978:ARG:HB2	3:J:1199:PHE:HZ	1.78	0.48
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.96	0.48
2:C:842:ASP:N	2:C:1045:GLY:O	2.47	0.48
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.95	0.48
3:D:1267:VAL:HB	3:D:1301:THR:OG1	2.14	0.48
3:D:218:THR:HA	3:D:221:ILE:HG22	1.96	0.48
1:G:177:TYR:O	1:G:178:SER:HB2	2.12	0.48
1:A:66:HIS:CE1	1:A:69:SER:HB3	2.49	0.48
2:C:145:ILE:HB	2:C:456:VAL:HG22	1.96	0.48
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.95	0.48
2:C:677:ASN:OD1	3:D:779:ALA:HB1	2.12	0.48
3:D:103:GLY:HA3	3:D:244:VAL:HG22	1.95	0.48
3:D:1191:PRO:HB2	3:D:1194:ARG:HD3	1.94	0.48
2:I:50:GLU:HG2	2:I:73:TYR:HE1	1.78	0.48
2:I:897:PRO:HG3	3:J:77:ARG:HH22	1.78	0.48
3:J:45:ASN:HB3	3:J:48:THR:O	2.13	0.48
1:B:211:ILE:HD11	1:B:215:GLU:OE2	2.13	0.48
3:D:1280:VAL:HG21	3:D:1304:ARG:NE	2.25	0.48
1:H:48:LEU:HD21	3:J:535:ARG:HG3	1.95	0.48
1:H:97:GLU:OE1	1:H:147:GLN:HG3	2.14	0.48
2:I:1176:LEU:HD13	2:I:1180:MET:HG2	1.96	0.48
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.95	0.48
2:I:971:LEU:HG	2:I:1014:LEU:HD23	1.96	0.48
3:J:650:LYS:O	3:J:654:ILE:HG13	2.14	0.48
5:L:281:ARG:O	5:L:285:ARG:HG3	2.13	0.48
1:A:228:LEU:HD11	1:B:221:ALA:HB1	1.96	0.48
1:B:54:CYS:SG	1:B:148:ARG:HG2	2.53	0.48
1:B:31:LEU:HD11	1:B:39:LEU:HD12	1.96	0.48
3:D:751:ASP:OD2	3:D:752:GLY:N	2.46	0.48
5:F:448:ARG:NH1	5:F:501:ALA:O	2.35	0.48
1:A:316:MET:HG2	5:F:600:HIS:CE1	2.49	0.48
3:J:950:ILE:HG13	3:J:1020:TRP:CH2	2.48	0.48
3:D:1198:VAL:HG23	3:D:1204:VAL:HG11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:752:GLY:O	3:D:754:ILE:N	2.47	0.48
2:I:115:LYS:HE3	2:I:116:ASP:H	1.78	0.48
2:I:538:LEU:HD22	2:I:543:ALA:HB2	1.95	0.48
2:I:842:ASP:N	2:I:1045:GLY:O	2.46	0.48
3:J:1167:LYS:HE3	3:J:1168:GLU:H	1.78	0.48
3:J:474:LEU:HD23	4:K:28:ARG:HG2	1.96	0.48
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.95	0.48
5:F:602:SER:N	5:F:605:GLU:OE2	2.46	0.48
2:I:202:ARG:HH22	2:I:368:ARG:HH12	1.61	0.48
2:I:799:ASN:HA	2:I:1231:TYR:HA	1.95	0.48
3:J:16:GLU:HG3	3:J:17:PHE:HD2	1.78	0.48
3:J:863:LEU:HD11	3:J:901:ARG:HB3	1.96	0.48
5:L:316:PHE:HZ	5:L:334:SER:HA	1.79	0.48
3:D:749:LYS:HE2	3:D:753:SER:HB3	1.96	0.48
2:I:1065:LYS:HD2	2:I:1235:LEU:HD12	1.96	0.48
2:I:1254:VAL:HG13	2:I:1255:THR:H	1.78	0.48
3:J:275:ARG:HD3	3:J:298:MET:HB3	1.95	0.48
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.97	0.47
2:C:819:SER:HB2	2:C:1085:MET:HG3	1.96	0.47
3:D:189:LEU:HB3	3:D:234:PRO:HB2	1.96	0.47
3:D:45:ASN:HB3	3:D:48:THR:O	2.14	0.47
1:H:73:GLY:HA3	1:H:138:ALA:HB1	1.96	0.47
2:I:820:GLU:N	2:I:1080:ASN:O	2.47	0.47
2:I:850:ILE:HG13	2:I:1048:LYS:HE2	1.95	0.47
3:J:1078:LEU:HD13	3:J:1121:LEU:HD22	1.96	0.47
3:J:218:THR:HA	3:J:221:ILE:HG22	1.96	0.47
3:J:568:SER:OG	3:J:569:LEU:N	2.47	0.47
5:L:461:ASN:O	5:L:465:ARG:HG2	2.13	0.47
5:L:573:LEU:H	5:L:573:LEU:HD23	1.79	0.47
2:C:850:ILE:HG13	2:C:1048:LYS:HE2	1.95	0.47
3:D:1167:LYS:HE3	3:D:1168:GLU:H	1.77	0.47
3:D:422:LEU:HD13	3:D:471:PRO:HG3	1.97	0.47
4:E:60:ASN:HD21	4:E:63:ILE:HD13	1.78	0.47
2:I:936:ARG:NH2	2:I:1043:ALA:O	2.47	0.47
1:A:54:CYS:HA	1:A:148:ARG:HG3	1.96	0.47
3:D:694:SER:OG	3:D:738:ARG:NE	2.39	0.47
3:D:800:LEU:HB3	3:D:920:ALA:HB1	1.97	0.47
3:J:975:ILE:HD13	3:J:980:THR:HG21	1.95	0.47
1:A:102:LEU:HB3	1:A:142:MET:HG2	1.95	0.47
1:A:282:VAL:O	1:A:316:MET:N	2.46	0.47
2:C:820:GLU:N	2:C:1080:ASN:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:244:THR:O	5:F:247:GLU:HG2	2.15	0.47
5:F:583:THR:HG22	5:F:584:ARG:H	1.80	0.47
3:J:1295:ASN:HB2	3:J:1298:VAL:HB	1.95	0.47
3:J:338:PHE:CB	3:J:343:LEU:HB2	2.44	0.47
3:J:385:LEU:HD11	3:J:408:VAL:HG12	1.97	0.47
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	2.27	0.47
3:J:824:PRO:HD3	3:J:835:LEU:HB2	1.96	0.47
3:J:839:VAL:HG12	3:J:864:LEU:HD12	1.97	0.47
2:C:115:LYS:HE3	2:C:116:ASP:H	1.78	0.47
2:C:1336:ASN:N	3:D:23:ALA:O	2.35	0.47
5:F:165:PHE:HE2	5:F:217:ALA:HA	1.79	0.47
5:F:316:PHE:HZ	5:F:334:SER:HA	1.80	0.47
5:F:532:LEU:O	5:F:536:THR:HG23	2.14	0.47
5:F:573:LEU:H	5:F:573:LEU:HD23	1.79	0.47
1:H:101:THR:H	1:H:116:THR:HG22	1.80	0.47
2:I:402:ARG:NH2	2:I:419:ILE:O	2.47	0.47
3:J:1349:GLU:N	3:J:1349:GLU:OE2	2.35	0.47
3:J:749:LYS:HE2	3:J:753:SER:HB3	1.96	0.47
2:C:97:ARG:HB3	2:C:121:GLU:HB2	1.95	0.47
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.96	0.47
5:F:41:ILE:HA	5:F:44:ILE:HG23	1.97	0.47
2:I:242:VAL:HB	2:I:245:ARG:HD2	1.95	0.47
2:C:402:ARG:NH2	2:C:419:ILE:O	2.47	0.47
3:D:425:ARG:HE	3:D:427:PRO:HD2	1.80	0.47
3:J:282:LEU:HD21	5:L:410:ILE:HG12	1.96	0.47
5:L:466:ILE:HD13	5:L:486:ARG:HB3	1.97	0.47
3:D:615:LYS:HB2	3:D:616:PRO:HD3	1.97	0.47
3:D:905:ARG:HH21	3:D:907:HIS:CB	2.28	0.47
5:F:137:TYR:HE1	5:F:351:THR:HB	1.80	0.47
1:G:231:PHE:CE2	1:H:43:LEU:HD21	2.50	0.47
2:I:817:LEU:HD11	2:I:1080:ASN:HD22	1.79	0.47
2:I:250:THR:HA	2:I:268:ARG:HA	1.96	0.47
1:G:66:HIS:CD2	2:I:929:ILE:HG22	2.50	0.47
1:A:48:LEU:HA	1:A:180:VAL:HG21	1.97	0.47
2:C:400:VAL:HG21	2:C:452:ARG:NH1	2.30	0.47
3:D:1227:HIS:HB2	3:J:1293:GLU:HG2	1.96	0.47
6:C:2001:4OB:H7	3:D:774:ILE:HG13	1.97	0.47
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.96	0.47
2:C:202:ARG:HH22	2:C:368:ARG:HH12	1.62	0.47
2:C:238:GLN:HB3	2:C:284:LEU:HD11	1.97	0.47
3:D:568:SER:OG	3:D:569:LEU:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1122:LYS:HG2	2:I:1229:TYR:CE1	2.49	0.47
3:J:205:LEU:HD23	3:J:217:LEU:HB3	1.97	0.47
3:J:425:ARG:HE	3:J:427:PRO:HD2	1.80	0.47
3:D:1239:ASP:OD1	3:D:1242:ARG:NH2	2.47	0.46
3:D:205:LEU:HD23	3:D:217:LEU:HB3	1.97	0.46
1:G:228:LEU:C	1:G:230:ALA:H	2.18	0.46
2:I:578:TYR:HB3	2:I:590:PRO:HG2	1.97	0.46
3:J:591:ILE:HG13	3:J:604:MET:HE2	1.97	0.46
5:L:299:LYS:HA	5:L:302:PHE:HB3	1.97	0.46
1:B:97:GLU:OE1	1:B:147:GLN:HG3	2.14	0.46
2:C:971:LEU:HG	2:C:1014:LEU:HD23	1.96	0.46
2:C:21:VAL:HG11	2:C:592:ARG:HD2	1.97	0.46
2:C:591:TYR:HD2	2:C:606:LEU:HD13	1.80	0.46
2:C:799:ASN:HA	2:C:1231:TYR:HA	1.96	0.46
1:H:16:ILE:HG13	1:H:26:VAL:HG22	1.95	0.46
2:I:206:ALA:O	2:I:209:ILE:HG22	2.15	0.46
5:L:492:ASP:HB2	5:L:495:ARG:HH12	1.80	0.46
1:A:10:LYS:HE2	1:B:229:GLU:HB3	1.98	0.46
3:J:103:GLY:HA3	3:J:244:VAL:HG22	1.96	0.46
3:J:695:LYS:HA	3:J:695:LYS:HD3	1.73	0.46
4:K:73:GLN:HA	4:K:76:GLU:HB3	1.97	0.46
5:L:287:ILE:HG12	5:L:337:VAL:HG13	1.97	0.46
2:C:1280:ALA:HB1	3:D:918:ILE:HG22	1.97	0.46
2:C:217:THR:HG23	2:C:351:LEU:HD13	1.97	0.46
2:C:724:VAL:HG11	2:C:727:VAL:HG22	1.97	0.46
2:C:813:GLU:HB2	3:D:461:PHE:HB2	1.97	0.46
3:D:1319:PHE:CE2	3:D:1342:ASP:HB2	2.50	0.46
3:J:1060:VAL:HG22	3:J:1106:ILE:HG23	1.97	0.46
3:J:35:PHE:HD1	3:J:101:ARG:HD3	1.80	0.46
3:J:587:LEU:HD11	3:J:608:CYS:HA	1.96	0.46
3:J:77:ARG:HG3	3:J:79:LYS:H	1.80	0.46
5:L:137:TYR:HE1	5:L:351:THR:HB	1.81	0.46
3:D:405:GLU:O	3:D:408:VAL:HG22	2.16	0.46
3:D:412:LEU:HA	3:D:415:VAL:HG22	1.97	0.46
3:D:548:VAL:HG12	3:D:550:VAL:HG13	1.98	0.46
3:D:860:ARG:HB3	3:D:861:ASN:H	1.53	0.46
1:H:56:VAL:HG22	1:H:144:ILE:HD11	1.96	0.46
3:J:120:LEU:HD12	5:L:43:ASP:HB3	1.96	0.46
3:J:325:LYS:HD3	5:L:508:GLU:CG	2.45	0.46
1:A:79:LEU:HD11	2:C:693:LEU:HD21	1.98	0.46
2:C:680:LEU:O	2:C:684:ASN:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1230:THR:OG1	3:D:1257:VAL:HG11	2.16	0.46
3:J:1170:LYS:C	3:J:1172:LYS:H	2.19	0.46
3:J:502:PRO:HB2	3:J:507:VAL:HG12	1.98	0.46
1:A:54:CYS:O	1:A:146:VAL:HG13	2.16	0.46
3:D:115:TRP:CE2	3:D:1329:THR:HG23	2.51	0.46
3:D:35:PHE:HD1	3:D:101:ARG:HD3	1.80	0.46
5:F:287:ILE:HG12	5:F:337:VAL:HG13	1.98	0.46
1:G:102:LEU:HB3	1:G:142:MET:HG2	1.97	0.46
1:G:79:LEU:CD1	2:I:693:LEU:HD21	2.45	0.46
1:B:56:VAL:HG22	1:B:144:ILE:HD11	1.98	0.46
1:B:73:GLY:HA3	1:B:138:ALA:HB1	1.96	0.46
2:C:149:LEU:HD11	2:C:451:ARG:HB3	1.97	0.46
2:C:509:SER:HB3	2:C:512:SER:HB3	1.97	0.46
4:E:60:ASN:ND2	4:E:63:ILE:HD13	2.30	0.46
1:G:172:LEU:HD12	1:G:172:LEU:H	1.81	0.46
3:J:266:ASN:O	3:J:270:ARG:HB2	2.15	0.46
1:A:177:TYR:O	1:A:178:SER:HB2	2.14	0.46
3:D:1295:ASN:HB2	3:D:1298:VAL:HB	1.98	0.46
3:D:68:TYR:HA	3:D:92:VAL:HG23	1.96	0.46
3:D:735:ALA:O	3:D:738:ARG:HB3	2.16	0.46
5:F:313:ASP:OD1	5:F:338:HIS:NE2	2.49	0.46
2:I:10:ARG:NH1	2:I:697:LYS:HD3	2.31	0.46
2:I:705:GLU:HB2	2:I:794:LEU:HB3	1.98	0.46
3:J:422:LEU:HD13	3:J:471:PRO:HG3	1.98	0.46
3:J:79:LYS:HG3	3:J:80:HIS:N	2.31	0.46
5:L:165:PHE:HE2	5:L:217:ALA:HA	1.79	0.46
5:L:493:LYS:HA	5:L:496:LYS:HE2	1.98	0.46
1:A:93:GLN:HB2	1:A:120:ASP:OD2	2.16	0.46
1:B:48:LEU:HD12	1:B:183:ILE:HD11	1.98	0.46
2:C:1336:ASN:O	3:D:23:ALA:N	2.46	0.46
2:C:170:VAL:HG23	2:C:171:LEU:N	2.31	0.46
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.97	0.46
3:D:120:LEU:HD23	5:F:47:MET:SD	2.55	0.46
3:D:385:LEU:HD11	3:D:408:VAL:HG12	1.96	0.46
1:G:10:LYS:HB3	1:G:10:LYS:HE3	1.71	0.46
2:I:1312:ASN:OD1	2:I:1314:GLN:HG3	2.16	0.46
2:I:146:VAL:HG13	2:I:529:ARG:HB3	1.97	0.46
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.98	0.46
3:J:50:LYS:HB3	3:J:71:LEU:HD21	1.98	0.46
2:C:840:SER:O	2:C:1047:LEU:N	2.49	0.45
2:C:1159:VAL:HB	2:C:1160:ASP:H	1.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:217:THR:HG23	2:I:351:LEU:HD13	1.97	0.45
2:I:448:LEU:HB2	2:I:553:THR:HB	1.97	0.45
2:I:697:LYS:HE2	2:I:697:LYS:HB3	1.82	0.45
3:J:1286:LYS:HD2	3:J:1290:ARG:NH2	2.31	0.45
2:C:206:ALA:O	2:C:209:ILE:HG22	2.16	0.45
2:C:448:LEU:HB2	2:C:553:THR:HB	1.97	0.45
5:F:493:LYS:HA	5:F:496:LYS:HE2	1.97	0.45
5:F:572:THR:O	5:F:576:VAL:HG23	2.16	0.45
1:G:68:TYR:OH	2:I:1057:LYS:HB2	2.16	0.45
2:I:1281:TYR:CD1	3:J:484:MET:HG2	2.51	0.45
2:I:453:ILE:HD12	2:I:587:LEU:HD21	1.98	0.45
3:J:950:ILE:HB	3:J:1018:ALA:HB3	1.99	0.45
3:J:1095:MET:HA	3:J:1096:PRO:HD3	1.83	0.45
3:J:1244:GLN:HE21	3:J:1244:GLN:HB3	1.58	0.45
3:J:246:PRO:HA	3:J:247:PRO:HD3	1.80	0.45
1:B:101:THR:H	1:B:116:THR:HG22	1.80	0.45
1:B:221:ALA:O	1:B:224:LEU:HB3	2.16	0.45
6:C:2001:4OB:H1	3:D:774:ILE:HG12	1.97	0.45
3:D:190:LYS:HD3	3:D:235:GLU:HG2	1.98	0.45
3:D:712:GLN:CD	3:D:712:GLN:H	2.19	0.45
2:I:322:LEU:O	2:I:326:SER:OG	2.30	0.45
2:I:28:LEU:HD21	2:I:524:ILE:HG13	1.98	0.45
3:J:735:ALA:O	3:J:738:ARG:HB3	2.16	0.45
5:L:561:MET:HG3	5:L:571:TYR:CD2	2.51	0.45
5:L:572:THR:O	5:L:576:VAL:HG23	2.16	0.45
1:B:78:ILE:O	1:B:82:LEU:HG	2.16	0.45
2:C:56:VAL:HG11	2:C:468:LEU:HB3	1.97	0.45
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.98	0.45
3:D:598:LYS:O	3:D:601:ILE:HG22	2.16	0.45
3:D:611:ILE:HG22	3:D:612:LEU:HD12	1.98	0.45
3:D:885:VAL:HG12	3:D:894:VAL:HG11	1.98	0.45
3:D:133:ARG:HD3	5:F:88:GLU:O	2.16	0.45
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.56	0.45
3:J:258:GLY:HA3	5:L:499:LYS:HD3	1.98	0.45
5:L:97:PRO:HA	5:L:100:MET:HG3	1.98	0.45
1:A:64:VAL:HG11	1:A:78:ILE:HG21	1.99	0.45
3:D:124:ILE:HG23	3:D:189:LEU:HD11	1.97	0.45
3:D:266:ASN:O	3:D:270:ARG:HB2	2.17	0.45
3:D:113:HIS:CE1	3:D:307:LEU:HD13	2.52	0.45
3:D:587:LEU:HD11	3:D:608:CYS:HA	1.99	0.45
3:D:709:ARG:C	3:D:711:GLY:H	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:190:LYS:HD3	3:J:235:GLU:HG2	1.98	0.45
4:K:60:ASN:HD21	4:K:63:ILE:HD13	1.81	0.45
2:C:1065:LYS:HD2	2:C:1235:LEU:HD12	1.97	0.45
2:C:1288:GLN:HE21	3:D:1355:ARG:HA	1.81	0.45
3:D:502:PRO:HB2	3:D:507:VAL:HG12	1.99	0.45
3:D:62:PHE:O	3:D:101:ARG:HD2	2.17	0.45
5:F:569:THR:OG1	5:F:570:ASP:N	2.48	0.45
1:G:64:VAL:HG11	1:G:78:ILE:HG21	1.99	0.45
2:I:1125:GLY:HA3	2:I:1179:GLY:HA2	1.98	0.45
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.80	0.45
3:J:1025:MET:SD	3:J:1124:ILE:HD12	2.57	0.45
3:J:115:TRP:CE2	3:J:1329:THR:HG23	2.51	0.45
3:J:198:CYS:O	3:J:202:ARG:HG3	2.16	0.45
1:A:172:LEU:HD12	1:A:172:LEU:H	1.82	0.45
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.98	0.45
3:D:1287:ILE:O	3:D:1291:GLU:HG3	2.16	0.45
1:G:228:LEU:CD1	1:H:221:ALA:HB1	2.45	0.45
2:I:183:TRP:HB2	2:I:199:ASP:HA	1.99	0.45
3:J:298:MET:SD	5:L:402:LEU:HB3	2.57	0.45
5:L:313:ASP:OD1	5:L:338:HIS:NE2	2.50	0.45
5:L:582:VAL:HG22	5:L:586:ARG:HG2	1.98	0.45
2:C:724:VAL:HA	2:C:734:ILE:HD13	1.99	0.45
3:D:1170:LYS:C	3:D:1172:LYS:H	2.19	0.45
3:D:1227:HIS:CD2	3:J:1293:GLU:HG2	2.52	0.45
3:D:50:LYS:HB3	3:D:71:LEU:HD21	1.99	0.45
2:I:746:ALA:HB3	2:I:971:LEU:HA	1.98	0.45
3:J:1078:LEU:HB3	3:J:1121:LEU:HD13	1.98	0.45
3:J:334:LYS:HA	3:J:334:LYS:HD2	1.57	0.45
3:J:405:GLU:O	3:J:408:VAL:HG22	2.16	0.45
3:J:611:ILE:HG22	3:J:612:LEU:HD12	1.99	0.45
4:K:60:ASN:ND2	4:K:63:ILE:HD13	2.32	0.45
2:C:196:VAL:HG12	2:C:206:ALA:HA	1.99	0.45
1:G:106:GLY:HA2	1:G:136:GLU:O	2.16	0.45
1:G:54:CYS:HA	1:G:148:ARG:HG3	1.98	0.45
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.97	0.45
3:J:1046:ILE:HD12	3:J:1059:LEU:HB3	1.99	0.45
3:J:264:ASP:OD2	3:J:264:ASP:N	2.50	0.45
3:J:598:LYS:O	3:J:601:ILE:HG22	2.17	0.45
3:J:62:PHE:O	3:J:101:ARG:HD2	2.17	0.45
3:J:950:ILE:HG13	3:J:1020:TRP:HH2	1.82	0.45
5:L:130:VAL:HB	5:L:365:MET:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:GLU:O	1:A:320:ASN:HB2	2.16	0.45
2:C:136:PHE:CE2	2:C:456:VAL:HG11	2.52	0.45
3:D:1146:GLU:HB3	3:D:1148:ARG:HG3	1.99	0.45
3:D:708:ASN:N	3:D:708:ASN:OD1	2.50	0.45
3:D:418:GLU:H	4:E:45:LYS:NZ	2.15	0.45
2:I:732:ILE:HD11	2:I:769:PRO:HB3	1.99	0.45
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.82	0.45
3:J:548:VAL:HG12	3:J:550:VAL:HG13	1.99	0.45
1:A:106:GLY:HA2	1:A:136:GLU:O	2.17	0.44
3:D:770:LEU:H	3:D:770:LEU:HD22	1.82	0.44
1:G:48:LEU:HA	1:G:180:VAL:HG21	2.00	0.44
2:I:1286:THR:N	3:J:479:GLU:OE2	2.44	0.44
3:J:294:ASN:HD22	5:L:406:GLN:NE2	2.15	0.44
5:L:412:LEU:HD13	5:L:435:ILE:HD11	1.98	0.44
5:L:547:VAL:HG12	5:L:598:LEU:HD22	1.99	0.44
3:D:37:GLU:HB2	3:D:104:HIS:CE1	2.52	0.44
5:F:605:GLU:HG3	5:F:605:GLU:H	1.53	0.44
1:H:221:ALA:O	1:H:224:LEU:HB3	2.16	0.44
3:J:35:PHE:CD1	3:J:101:ARG:HD3	2.53	0.44
3:J:694:SER:OG	3:J:738:ARG:NE	2.40	0.44
3:J:709:ARG:C	3:J:711:GLY:H	2.20	0.44
3:J:430:HIS:HA	3:J:921:GLN:HB3	1.98	0.44
5:L:234:THR:O	5:L:245:ALA:HB2	2.17	0.44
5:L:569:THR:OG1	5:L:570:ASP:N	2.50	0.44
3:D:1286:LYS:HD2	3:D:1290:ARG:NH2	2.32	0.44
3:D:16:GLU:HG3	3:D:1369:ARG:NH2	2.33	0.44
5:F:492:ASP:HB2	5:F:495:ARG:HH12	1.81	0.44
1:H:108:GLY:O	1:H:133:LEU:HB2	2.16	0.44
2:I:1323:PHE:CE1	3:J:1353:VAL:HG23	2.52	0.44
6:I:2001:4OB:H7	3:J:774:ILE:HG12	1.99	0.44
2:I:56:VAL:HG11	2:I:468:LEU:HB3	2.00	0.44
3:J:615:LYS:HB2	3:J:616:PRO:HD3	1.99	0.44
1:A:12:ARG:H	1:A:30:PRO:HD2	1.82	0.44
2:I:808:ASN:OD1	2:I:1216:ARG:NH2	2.50	0.44
3:J:412:LEU:HA	3:J:415:VAL:HG22	2.00	0.44
3:J:421:VAL:HG13	3:J:439:PRO:HG3	1.99	0.44
1:A:231:PHE:HE1	1:B:39:LEU:HD13	1.81	0.44
2:C:389:PHE:HB3	2:C:420:LEU:HD12	1.99	0.44
5:F:299:LYS:HA	5:F:302:PHE:HB3	1.98	0.44
5:F:602:SER:H	5:F:605:GLU:HG3	1.80	0.44
2:I:591:TYR:HD2	2:I:606:LEU:HD13	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:122:SER:O	3:J:126:LEU:HG	2.18	0.44
3:J:1287:ILE:O	3:J:1291:GLU:HG3	2.18	0.44
3:J:679:TYR:CZ	3:J:683:ILE:HD12	2.53	0.44
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.48	0.44
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.32	0.44
3:D:1280:VAL:O	3:D:1284:ARG:HB3	2.18	0.44
3:D:1343:GLU:HB3	3:D:1345:ARG:HD3	2.00	0.44
3:J:113:HIS:CE1	3:J:307:LEU:HD13	2.52	0.44
3:J:1239:ASP:OD1	3:J:1242:ARG:NH2	2.49	0.44
2:C:678:ARG:HG3	2:C:1108:ASN:HD22	1.82	0.44
2:C:383:SER:O	2:C:387:ASN:HB2	2.18	0.44
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.32	0.44
2:C:901:LEU:HB2	5:F:565:ILE:HD11	1.99	0.44
3:D:290:ILE:HD12	3:D:290:ILE:H	1.82	0.44
3:D:863:LEU:HD11	3:D:901:ARG:HB3	1.98	0.44
5:F:362:ASN:HB2	5:F:365:MET:HE2	1.99	0.44
5:F:44:ILE:HA	5:F:47:MET:HB2	1.99	0.44
1:G:58:GLU:HB2	1:G:145:LYS:HB3	1.98	0.44
1:G:229:GLU:OE1	1:H:10:LYS:HD3	2.17	0.44
2:I:113:THR:OG1	2:I:116:ASP:OD2	2.25	0.44
2:I:26:TYR:CE2	2:I:32:LEU:HD12	2.52	0.44
2:I:660:VAL:HG11	3:J:769:VAL:HG13	1.99	0.44
2:I:680:LEU:O	2:I:684:ASN:HB2	2.17	0.44
2:I:724:VAL:HG11	2:I:727:VAL:HG22	1.99	0.44
2:I:782:VAL:HG11	2:I:792:GLY:HA2	2.00	0.44
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.99	0.44
2:I:549:ASP:OD2	3:J:777:HIS:ND1	2.49	0.44
3:D:349:TYR:HE2	3:D:379:PRO:HG2	1.83	0.44
3:D:421:VAL:HG13	3:D:439:PRO:HG3	1.99	0.44
5:F:249:ILE:O	5:F:252:LEU:HB3	2.17	0.44
2:I:299:LYS:HE2	2:I:299:LYS:HB2	1.61	0.44
3:J:1156:LEU:HB3	3:J:1207:GLY:HA2	2.00	0.44
3:J:1319:PHE:CE2	3:J:1342:ASP:HB2	2.53	0.44
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.50	0.44
3:D:1205:GLU:O	3:D:1208:ASP:HB2	2.18	0.44
3:D:77:ARG:NE	5:F:569:THR:HA	2.33	0.44
3:D:905:ARG:HH21	3:D:907:HIS:HB3	1.83	0.44
3:D:614:LEU:HD23	4:E:7:GLN:HB2	2.00	0.44
5:F:234:THR:O	5:F:245:ALA:HB2	2.18	0.44
1:G:39:LEU:HD23	1:G:39:LEU:HA	1.84	0.44
5:L:249:ILE:O	5:L:252:LEU:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:346:GLN:O	5:L:350:GLU:HG3	2.18	0.44
1:B:102:LEU:HD23	1:B:115:ILE:HG23	2.00	0.43
3:D:1293:GLU:HB3	3:D:1294:ALA:H	1.69	0.43
3:D:264:ASP:N	3:D:264:ASP:OD2	2.51	0.43
3:D:930:LEU:HD11	3:D:1241:TYR:CE2	2.53	0.43
2:I:1159:VAL:HB	2:I:1160:ASP:H	1.60	0.43
2:I:60:GLN:HB3	2:I:67:GLU:HG3	2.00	0.43
3:J:1205:GLU:O	3:J:1208:ASP:HB2	2.17	0.43
3:J:751:ASP:OD2	3:J:752:GLY:N	2.51	0.43
3:J:756:GLU:H	3:J:756:GLU:HG2	1.55	0.43
3:J:885:VAL:HG12	3:J:894:VAL:HG11	1.99	0.43
2:C:670:PHE:HZ	2:C:1117:LEU:HD13	1.83	0.43
2:C:1282:GLY:O	3:D:1361:THR:N	2.50	0.43
2:C:453:ILE:HD12	2:C:587:LEU:HD21	2.00	0.43
3:D:557:LYS:HE3	3:D:557:LYS:HB2	1.79	0.43
5:F:346:GLN:O	5:F:350:GLU:HG3	2.18	0.43
3:J:511:TYR:OH	3:J:515:ARG:NH1	2.52	0.43
1:A:152:TYR:CG	2:C:824:GLN:HG2	2.54	0.43
2:C:942:ASP:OD2	2:C:1048:LYS:NZ	2.34	0.43
3:D:122:SER:O	3:D:126:LEU:HG	2.18	0.43
3:D:810:THR:HG23	3:D:811:GLU:H	1.83	0.43
5:F:559:LEU:HA	5:F:559:LEU:HD12	1.83	0.43
2:I:170:VAL:HG23	2:I:171:LEU:N	2.32	0.43
2:I:778:GLU:O	2:I:781:ASP:HB2	2.18	0.43
5:L:136:GLU:OE1	5:L:364:ARG:NH2	2.51	0.43
1:B:100:LEU:HB2	1:B:144:ILE:HG23	2.01	0.43
2:C:237:LEU:H	2:C:237:LEU:HD22	1.83	0.43
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.48	0.43
2:C:996:ARG:HD3	2:C:996:ARG:HA	1.90	0.43
3:D:712:GLN:N	3:D:712:GLN:CD	2.71	0.43
3:D:430:HIS:HA	3:D:921:GLN:HB3	2.00	0.43
2:I:17:LYS:HE3	2:I:1154:ASP:HB3	2.00	0.43
2:I:524:ILE:HG21	2:I:708:VAL:HG13	2.00	0.43
3:J:1193:TRP:HB2	3:J:1194:ARG:NH1	2.33	0.43
3:J:1341:ARG:HH22	3:J:1373:ARG:HH21	1.65	0.43
3:J:30:ILE:HG23	3:J:243:PRO:HG3	1.99	0.43
2:I:1267:GLY:HA3	3:J:347:VAL:O	2.18	0.43
2:I:1253:LEU:HA	5:L:525:ASP:HB2	2.01	0.43
1:A:58:GLU:HB2	1:A:145:LYS:HB3	2.00	0.43
1:B:108:GLY:O	1:B:133:LEU:HB2	2.18	0.43
1:B:41:ASN:ND2	2:C:1217:THR:HA	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:17:LYS:HE3	2:C:1154:ASP:HB3	2.00	0.43
2:C:739:ASP:OD1	2:C:739:ASP:N	2.38	0.43
3:D:30:ILE:HG23	3:D:243:PRO:HG3	1.98	0.43
5:F:215:GLU:HG2	5:F:218:ARG:HH21	1.82	0.43
5:F:561:MET:SD	5:F:576:VAL:HG13	2.59	0.43
1:H:102:LEU:HD12	1:H:142:MET:HG2	2.00	0.43
3:J:426:ALA:HB3	3:J:427:PRO:HD3	2.00	0.43
3:J:709:ARG:O	3:J:711:GLY:N	2.51	0.43
3:J:800:LEU:O	3:J:803:VAL:HG12	2.18	0.43
2:C:10:ARG:HA	2:C:1172:LEU:HD23	2.01	0.43
2:C:1323:PHE:CE1	3:D:1353:VAL:HG23	2.53	0.43
2:C:705:GLU:HB2	2:C:794:LEU:HB3	2.00	0.43
3:D:1156:LEU:HB3	3:D:1207:GLY:HA2	1.99	0.43
3:D:355:ILE:HD13	3:D:466:MET:HG3	2.00	0.43
3:D:872:LEU:O	3:D:877:VAL:HG12	2.18	0.43
1:H:99:ILE:HD11	1:H:143:ARG:HB3	2.00	0.43
1:H:78:ILE:O	1:H:82:LEU:HG	2.19	0.43
2:I:1247:SER:HB3	3:J:375:GLU:O	2.19	0.43
2:I:26:TYR:O	2:I:29:SER:HB2	2.18	0.43
2:I:700:VAL:HG13	2:I:1117:LEU:HD22	2.00	0.43
3:J:1034:PHE:HA	3:J:1114:GLN:HA	2.01	0.43
3:J:1280:VAL:O	3:J:1284:ARG:HB3	2.19	0.43
2:I:1280:ALA:HB1	3:J:918:ILE:HG22	2.00	0.43
5:L:289:LYS:HE2	5:L:289:LYS:HB3	1.88	0.43
1:A:12:ARG:HG3	1:B:230:ALA:HB1	2.01	0.43
1:A:39:LEU:HA	1:A:39:LEU:HD23	1.83	0.43
2:C:1122:LYS:HG2	2:C:1229:TYR:CZ	2.54	0.43
2:C:524:ILE:HG21	2:C:708:VAL:HG13	1.99	0.43
2:C:778:GLU:O	2:C:781:ASP:HB2	2.19	0.43
3:D:77:ARG:HD2	3:D:78:LEU:H	1.84	0.43
1:G:102:LEU:HD22	1:G:103:ASN:H	1.84	0.43
3:J:367:GLY:HA3	3:J:448:GLN:HB2	2.01	0.43
2:I:1289:GLU:OE2	3:J:473:THR:HG22	2.19	0.43
3:J:810:THR:HG23	3:J:811:GLU:H	1.83	0.43
2:I:1302:THR:HG22	5:L:531:PRO:HB3	2.01	0.43
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.59	0.43
2:C:887:VAL:HB	2:C:913:VAL:HG21	2.00	0.43
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.53	0.43
3:D:1163:VAL:HG23	3:D:1177:ILE:HA	2.01	0.43
3:D:426:ALA:HB3	3:D:427:PRO:HD3	2.01	0.43
2:I:10:ARG:HA	2:I:1172:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:657:THR:OG1	2:I:1187:PHE:HB2	2.18	0.43
5:L:482:GLU:HG2	5:L:486:ARG:HH22	1.84	0.43
1:B:80:GLU:HG3	3:D:551:ARG:NH2	2.33	0.43
3:D:800:LEU:O	3:D:803:VAL:HG12	2.18	0.43
1:G:66:HIS:CE1	1:G:69:SER:HB3	2.54	0.43
2:I:670:PHE:HZ	2:I:1117:LEU:HD13	1.83	0.43
2:I:1122:LYS:HG2	2:I:1229:TYR:CZ	2.53	0.43
2:I:518:ASN:O	2:I:691:PRO:HD3	2.19	0.43
2:C:69:GLN:HE21	2:C:69:GLN:HB3	1.67	0.43
2:C:758:ARG:HD3	2:C:835:GLU:HB2	2.01	0.43
2:C:897:PRO:CG	3:D:77:ARG:HH22	2.31	0.43
5:F:136:GLU:OE1	5:F:364:ARG:NH2	2.52	0.43
2:I:383:SER:O	2:I:387:ASN:HB2	2.19	0.43
3:J:1230:THR:OG1	3:J:1257:VAL:HG11	2.19	0.43
3:J:203:GLU:O	3:J:207:GLU:HG2	2.19	0.43
3:J:697:MET:O	3:J:701:LEU:HB2	2.19	0.43
3:J:701:LEU:HD13	3:J:723:TYR:HB2	2.01	0.43
5:L:507:MET:HG2	5:L:520:GLY:HA3	2.00	0.43
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.48	0.42
1:B:99:ILE:HD11	1:B:143:ARG:HB3	2.01	0.42
1:A:79:LEU:CD1	2:C:693:LEU:HD21	2.49	0.42
3:D:161:THR:HG22	3:D:164:GLN:CD	2.39	0.42
3:D:394:ILE:CG2	5:F:536:THR:HA	2.49	0.42
3:D:701:LEU:HD13	3:D:723:TYR:HB2	2.00	0.42
1:G:35:PHE:HA	1:G:35:PHE:HD1	1.70	0.42
1:H:11:PRO:HB3	1:H:30:PRO:O	2.18	0.42
2:I:1282:GLY:HA3	4:K:17:PHE:CE1	2.54	0.42
2:I:149:LEU:HB2	2:I:530:ILE:CG2	2.49	0.42
3:J:438:GLU:HA	3:J:439:PRO:HD3	1.85	0.42
3:J:573:THR:OG1	3:J:576:ARG:HG3	2.19	0.42
3:D:497:GLU:HA	3:D:498:PRO:HD3	1.85	0.42
3:J:349:TYR:HE2	3:J:379:PRO:HG2	1.84	0.42
3:J:708:ASN:N	3:J:708:ASN:OD1	2.50	0.42
5:L:582:VAL:CG2	5:L:586:ARG:HG2	2.49	0.42
5:L:583:THR:HB	5:L:584:ARG:HG2	2.01	0.42
1:B:64:VAL:HG21	1:B:69:SER:CB	2.49	0.42
2:C:98:VAL:HG21	2:C:124:MET:HE3	2.01	0.42
3:D:1287:ILE:HG13	3:D:1288:ALA:N	2.35	0.42
3:D:418:GLU:HB2	4:E:45:LYS:HB2	2.01	0.42
3:D:557:LYS:HA	3:D:563:LEU:HA	2.02	0.42
3:D:709:ARG:O	3:D:711:GLY:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:48:LEU:HA	1:H:180:VAL:HG21	2.01	0.42
2:I:196:VAL:HG12	2:I:206:ALA:HA	2.00	0.42
2:I:238:GLN:HB3	2:I:284:LEU:HD11	2.00	0.42
2:I:360:LEU:HB2	2:I:378:ARG:HH21	1.84	0.42
2:I:389:PHE:HB3	2:I:420:LEU:HD12	2.00	0.42
2:I:634:VAL:HG13	2:I:636:CYS:SG	2.59	0.42
2:I:710:VAL:HA	2:I:715:THR:HG21	2.01	0.42
3:D:1293:GLU:HG2	3:J:1227:HIS:HB2	2.01	0.42
3:D:1226:VAL:HB	3:J:1293:GLU:H	1.83	0.42
3:J:1348:LYS:HA	3:J:1348:LYS:HD2	1.85	0.42
3:J:1368:ASP:OD1	3:J:1371:ARG:NH2	2.52	0.42
3:J:987:GLU:HG3	3:J:987:GLU:H	1.64	0.42
2:C:38:PHE:HB2	2:C:457:GLY:CA	2.48	0.42
2:C:83:GLN:O	2:C:87:ILE:HG13	2.19	0.42
2:C:660:VAL:HG11	3:D:769:VAL:HG13	2.01	0.42
4:E:66:VAL:HG22	4:E:69:ARG:HH21	1.84	0.42
5:F:22:LEU:H	5:F:54:GLN:CB	2.33	0.42
2:I:519:ASN:HD21	2:I:796:LEU:HD23	1.84	0.42
2:I:964:LEU:HD22	2:I:1025:PHE:CG	2.54	0.42
3:J:425:ARG:HH12	3:J:464:ASP:CG	2.21	0.42
2:I:1101:LEU:HD13	3:J:504:GLN:HB2	2.01	0.42
4:K:66:VAL:HG22	4:K:69:ARG:HH21	1.85	0.42
5:L:215:GLU:HG2	5:L:218:ARG:HH21	1.82	0.42
1:B:61:ILE:HG21	1:B:78:ILE:HD13	2.02	0.42
2:C:964:LEU:HD22	2:C:1025:PHE:CG	2.54	0.42
2:C:360:LEU:HB2	2:C:378:ARG:HH21	1.85	0.42
2:C:499:SER:O	2:C:503:LYS:HB2	2.20	0.42
2:C:720:ARG:HA	2:C:779:ARG:HG3	2.01	0.42
3:D:505:ASP:HB2	3:D:629:PHE:HE1	1.85	0.42
5:F:412:LEU:HD13	5:F:435:ILE:HD11	2.00	0.42
2:I:1294:LYS:HD3	3:J:472:LEU:HG	2.00	0.42
2:I:18:ARG:HA	2:I:19:PRO:HD3	1.92	0.42
2:I:203:LYS:CB	5:L:29:ASP:HB2	2.49	0.42
2:I:538:LEU:H	2:I:538:LEU:HG	1.64	0.42
2:I:887:VAL:HB	2:I:913:VAL:CG2	2.49	0.42
5:L:399:LEU:HA	5:L:399:LEU:HD12	1.85	0.42
5:L:580:PHE:C	5:L:582:VAL:H	2.23	0.42
1:B:89:ALA:HB3	1:B:124:VAL:HG12	2.02	0.42
1:B:112:ALA:HB2	1:B:128:HIS:HB3	2.00	0.42
1:B:84:ASN:O	1:B:128:HIS:HE1	2.03	0.42
2:C:1125:GLY:HA3	2:C:1179:GLY:HA2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:334:LYS:HD2	3:D:334:LYS:HA	1.58	0.42
3:D:697:MET:O	3:D:701:LEU:HB2	2.19	0.42
1:H:100:LEU:HB2	1:H:144:ILE:HG23	2.01	0.42
1:H:151:GLY:O	1:H:177:TYR:HD2	2.03	0.42
2:I:660:VAL:HG13	2:I:661:VAL:HG13	2.00	0.42
2:I:806:PRO:O	3:J:633:ALA:HA	2.19	0.42
3:J:1198:VAL:HB	3:J:1210:ILE:HA	2.01	0.42
2:C:211:ARG:NH1	2:C:357:ASN:O	2.52	0.42
2:C:518:ASN:O	2:C:691:PRO:HD3	2.19	0.42
1:G:182:ARG:HB3	1:G:206:GLU:HB3	2.02	0.42
1:G:182:ARG:C	1:G:183:ILE:HD12	2.40	0.42
2:I:616:ILE:HG13	2:I:652:TYR:HB2	2.01	0.42
2:I:1276:TRP:HE1	3:J:1348:LYS:NZ	2.18	0.42
3:J:355:ILE:HD13	3:J:466:MET:HG3	2.01	0.42
5:L:314:THR:O	5:L:318:ALA:HB3	2.20	0.42
1:A:228:LEU:HD21	1:B:224:LEU:HD23	2.01	0.42
2:C:1080:ASN:HA	2:C:1081:PRO:HD3	1.96	0.42
2:C:1247:SER:O	3:D:348:ASP:HB3	2.20	0.42
2:C:60:GLN:HB3	2:C:67:GLU:HG3	2.01	0.42
2:C:1267:GLY:HA3	3:D:347:VAL:O	2.20	0.42
3:D:425:ARG:HH12	3:D:464:ASP:CG	2.23	0.42
3:D:490:ILE:HA	3:D:500:ILE:HD11	2.02	0.42
2:I:156:PHE:CE2	2:I:158:ASP:HB2	2.54	0.42
2:I:232:ILE:HG12	2:I:237:LEU:HD13	2.02	0.42
3:J:1163:VAL:HG23	3:J:1177:ILE:HA	2.02	0.42
3:J:901:ARG:HD2	3:J:906:GLY:O	2.19	0.42
5:L:441:ARG:NH1	5:L:445:ASP:OD1	2.50	0.42
1:A:41:ASN:HB2	1:A:185:TYR:OH	2.19	0.42
2:C:1276:TRP:HE1	3:D:1348:LYS:NZ	2.17	0.42
3:D:13:LYS:HD3	3:D:13:LYS:HA	1.72	0.42
2:C:1338:GLU:N	3:D:21:LYS:O	2.34	0.42
3:D:450:HIS:HA	3:D:451:PRO:HD3	1.85	0.42
5:F:484:ALA:HB1	5:F:491:GLU:HB2	2.02	0.42
5:F:507:MET:HG2	5:F:520:GLY:HA3	2.01	0.42
2:I:169:LYS:O	2:I:170:VAL:HG22	2.20	0.42
2:I:720:ARG:HA	2:I:779:ARG:HG3	2.01	0.42
3:J:1036:ARG:HG2	3:J:1037:PHE:H	1.85	0.42
5:L:124:GLU:O	5:L:128:ASN:HB2	2.20	0.42
5:L:454:VAL:HA	5:L:457:ILE:HD12	2.02	0.42
2:C:156:PHE:CE2	2:C:158:ASP:HB2	2.55	0.42
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:355:ILE:HG22	3:D:447:ILE:HB	2.01	0.42
3:D:385:LEU:HD23	3:D:385:LEU:HA	1.92	0.42
3:D:901:ARG:HD2	3:D:906:GLY:O	2.20	0.42
2:I:661:VAL:HB	2:I:665:ALA:HB3	2.01	0.42
2:I:887:VAL:HB	2:I:913:VAL:HG21	2.01	0.42
2:I:929:ILE:HD13	2:I:1055:ALA:HB2	2.01	0.42
3:J:1287:ILE:HG13	3:J:1288:ALA:N	2.34	0.42
3:J:290:ILE:HD12	3:J:290:ILE:H	1.85	0.42
3:J:974:VAL:HG21	3:J:1118:GLY:HA2	2.02	0.42
2:C:1059:ARG:HB2	2:C:1060:ILE:H	1.74	0.41
2:C:660:VAL:HG13	2:C:661:VAL:HG13	2.02	0.41
3:D:527:LEU:HD22	3:D:533:ALA:HA	2.02	0.41
1:G:31:LEU:CD1	1:G:201:LEU:HB2	2.50	0.41
2:I:1161:LEU:HA	2:I:1161:LEU:HD12	1.70	0.41
2:I:356:THR:HG21	2:I:362:ALA:HA	2.02	0.41
2:I:617:ALA:HA	2:I:636:CYS:SG	2.60	0.41
3:J:1146:GLU:HB3	3:J:1148:ARG:HG3	2.01	0.41
3:J:872:LEU:O	3:J:877:VAL:HG12	2.19	0.41
1:A:51:MET:HE3	1:A:51:MET:HB3	1.93	0.41
3:D:1198:VAL:HB	3:D:1210:ILE:HA	2.02	0.41
3:D:338:PHE:CB	3:D:343:LEU:HB2	2.50	0.41
3:D:794:GLY:O	3:D:797:THR:OG1	2.26	0.41
5:F:119:ILE:O	5:F:123:ILE:HG13	2.20	0.41
2:I:1257:GLN:OE1	3:J:340:GLN:NE2	2.53	0.41
2:I:32:LEU:HD23	2:I:32:LEU:HA	1.91	0.41
2:I:98:VAL:HG21	2:I:124:MET:HE3	2.02	0.41
2:I:996:ARG:HA	2:I:996:ARG:HD3	1.89	0.41
3:J:1027:VAL:HG21	3:J:1122:ALA:HB3	2.02	0.41
3:J:557:LYS:HA	3:J:563:LEU:HA	2.02	0.41
5:L:528:LEU:HD23	5:L:528:LEU:HA	1.92	0.41
2:C:593:LYS:HD3	2:C:652:TYR:CZ	2.56	0.41
3:D:1216:ALA:HA	3:D:1217:PRO:HD3	1.89	0.41
3:D:1349:GLU:N	3:D:1349:GLU:OE2	2.38	0.41
3:D:1355:ARG:NH1	3:D:1369:ARG:HH12	2.18	0.41
5:F:289:LYS:HB3	5:F:289:LYS:HE2	1.88	0.41
5:F:343:LYS:H	5:F:343:LYS:HD2	1.85	0.41
2:I:1010:GLN:O	2:I:1014:LEU:HD12	2.20	0.41
2:I:26:TYR:CE2	2:I:28:LEU:HB2	2.56	0.41
2:I:840:SER:O	2:I:1047:LEU:N	2.53	0.41
3:J:770:LEU:H	3:J:770:LEU:HD22	1.85	0.41
3:J:478:LEU:HB3	4:K:20:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:LEU:HD12	1:B:142:MET:HG2	2.02	0.41
2:C:101:ARG:HH21	2:C:118:LYS:HE3	1.85	0.41
2:C:357:ASN:ND2	2:C:358:ASP:OD2	2.53	0.41
2:C:561:ILE:HD11	2:C:665:ALA:HB1	2.01	0.41
2:C:616:ILE:HG13	2:C:652:TYR:HB2	2.02	0.41
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.36	0.41
3:D:482:ALA:HB3	4:E:20:VAL:HG22	2.03	0.41
5:F:561:MET:HG3	5:F:571:TYR:CD2	2.55	0.41
5:F:580:PHE:C	5:F:582:VAL:H	2.23	0.41
1:G:102:LEU:HD22	1:G:103:ASN:N	2.36	0.41
2:I:1062:PRO:HA	2:I:1076:ILE:HG23	2.02	0.41
2:I:499:SER:O	2:I:503:LYS:HB2	2.19	0.41
3:J:450:HIS:HA	3:J:451:PRO:HD3	1.85	0.41
3:J:474:LEU:HD12	3:J:474:LEU:HA	1.90	0.41
4:K:49:ILE:HA	4:K:52:ARG:HD3	2.02	0.41
5:L:420:GLU:OE1	5:L:423:ARG:NH2	2.50	0.41
1:A:182:ARG:C	1:A:183:ILE:HD12	2.40	0.41
2:C:183:TRP:HB2	2:C:199:ASP:HA	2.02	0.41
2:C:468:LEU:HA	2:C:471:VAL:HG12	2.02	0.41
2:C:617:ALA:HA	2:C:636:CYS:SG	2.61	0.41
2:C:925:SER:O	2:C:1056:VAL:HG13	2.21	0.41
3:D:1236:GLU:O	3:D:1240:VAL:HG23	2.21	0.41
3:D:203:GLU:O	3:D:207:GLU:HG2	2.20	0.41
4:E:4:VAL:HG22	4:E:5:THR:HG23	2.03	0.41
5:F:97:PRO:HA	5:F:100:MET:HG3	2.02	0.41
2:I:230:PHE:HE1	2:I:287:VAL:HG21	1.85	0.41
3:J:197:GLU:O	3:J:201:LEU:HG	2.20	0.41
3:J:654:ILE:O	3:J:658:GLU:HB2	2.21	0.41
5:L:245:ALA:O	5:L:249:ILE:HG13	2.20	0.41
1:A:31:LEU:CD1	1:A:201:LEU:HB2	2.48	0.41
2:C:1210:ILE:HG22	2:C:1211:ARG:H	1.85	0.41
2:C:959:ASP:O	2:C:963:GLU:HG2	2.21	0.41
3:D:591:ILE:HG13	3:D:604:MET:HE2	2.03	0.41
3:D:661:VAL:HG11	3:D:686:TRP:NE1	2.35	0.41
5:F:225:ARG:O	5:F:229:VAL:HG13	2.21	0.41
2:I:1210:ILE:HG22	2:I:1211:ARG:H	1.85	0.41
2:I:242:VAL:HA	2:I:243:PRO:HD3	1.93	0.41
2:I:555:TYR:HA	3:J:773:PHE:HE2	1.86	0.41
3:J:119:SER:O	3:J:121:PRO:HD2	2.21	0.41
3:J:361:LEU:HD22	3:J:365:GLN:HG3	2.01	0.41
3:J:572:THR:OG1	3:J:573:THR:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:759:ILE:HG22	3:J:761:ALA:O	2.21	0.41
1:B:20:SER:OG	1:B:21:SER:N	2.53	0.41
2:C:1109:ILE:HA	2:C:1109:ILE:HD12	1.86	0.41
2:C:169:LYS:O	2:C:170:VAL:HG22	2.21	0.41
2:C:53:PHE:O	2:C:57:PHE:HB2	2.21	0.41
2:C:634:VAL:HG13	2:C:636:CYS:SG	2.60	0.41
3:D:579:LEU:HD12	3:D:582:ILE:HD12	2.03	0.41
5:F:462:LYS:O	5:F:466:ILE:HG13	2.20	0.41
1:G:11:PRO:HD3	1:H:227:GLN:OE1	2.21	0.41
1:H:89:ALA:HB3	1:H:124:VAL:HG12	2.01	0.41
1:G:230:ALA:HB2	1:H:12:ARG:HA	2.03	0.41
1:H:64:VAL:HG21	1:H:69:SER:CB	2.50	0.41
1:H:65:LEU:HD13	1:H:65:LEU:O	2.21	0.41
2:I:357:ASN:ND2	2:I:358:ASP:OD2	2.53	0.41
2:I:374:GLU:HA	2:I:375:PRO:HD3	1.93	0.41
2:I:53:PHE:O	2:I:57:PHE:HB2	2.21	0.41
2:I:590:PRO:HB2	2:I:655:VAL:HG21	2.01	0.41
3:J:1237:VAL:HG13	3:J:1253:ILE:HD13	2.02	0.41
3:J:1319:PHE:CD2	3:J:1342:ASP:HB2	2.56	0.41
1:B:133:LEU:HD12	1:B:133:LEU:HA	1.92	0.41
2:C:551:HIS:CG	2:C:552:PRO:HD2	2.56	0.41
2:C:980:VAL:HG13	2:C:984:VAL:HB	2.02	0.41
2:I:149:LEU:HD11	2:I:451:ARG:HB3	2.03	0.41
2:I:593:LYS:HD3	2:I:652:TYR:CZ	2.55	0.41
2:I:658:GLN:O	2:I:661:VAL:HG22	2.21	0.41
3:J:137:ARG:HG2	3:J:143:SER:HB2	2.03	0.41
3:J:274:ASN:ND2	5:L:446:GLN:HB2	2.36	0.41
3:J:527:LEU:HD22	3:J:533:ALA:HA	2.02	0.41
3:J:70:CYS:SG	3:J:71:LEU:N	2.94	0.41
5:L:127:ILE:O	5:L:130:VAL:HG22	2.20	0.41
2:C:1010:GLN:O	2:C:1014:LEU:HD12	2.21	0.41
2:C:1211:ARG:O	2:C:1212:LEU:HD12	2.21	0.41
2:C:1313:HIS:HB2	3:D:474:LEU:HD13	2.02	0.41
1:A:75:GLN:HA	2:C:729:ALA:N	2.36	0.41
3:D:1319:PHE:CD2	3:D:1342:ASP:HB2	2.56	0.41
5:F:314:THR:O	5:F:318:ALA:HB3	2.21	0.41
2:I:213:LEU:HB3	2:I:422:LYS:CD	2.49	0.41
2:I:724:VAL:HA	2:I:734:ILE:HD13	2.02	0.41
3:J:1077:ALA:HA	3:J:1100:PHE:HA	2.02	0.41
3:J:930:LEU:HD11	3:J:1241:TYR:CE2	2.56	0.41
5:L:343:LYS:H	5:L:343:LYS:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:580:PHE:HD1	5:L:580:PHE:HA	1.71	0.41
1:A:10:LYS:HB3	1:A:10:LYS:HE3	1.79	0.41
1:B:191:ARG:HH22	3:D:409:TRP:CB	2.25	0.41
1:B:57:THR:O	1:B:173:VAL:HB	2.20	0.41
2:C:1179:GLY:O	2:C:1181:PRO:HD3	2.21	0.41
2:C:11:ILE:HA	2:C:11:ILE:HD13	1.88	0.41
2:C:171:LEU:HA	2:C:171:LEU:HD23	1.92	0.41
2:C:559:CYS:HA	2:C:560:PRO:HD3	1.89	0.41
3:D:19:ALA:HB2	3:D:1373:ARG:HH22	1.86	0.41
3:D:653:ILE:HD13	3:D:692:ARG:HB3	2.03	0.41
1:G:54:CYS:O	1:G:146:VAL:HG13	2.21	0.41
2:I:1262:LYS:HA	2:I:1262:LYS:HD3	1.83	0.41
2:I:145:ILE:HG13	2:I:512:SER:HB2	2.03	0.41
3:J:384:LYS:HD2	3:J:387:LEU:HD23	2.03	0.41
3:J:901:ARG:HA	3:J:908:ILE:HA	2.03	0.41
1:A:145:LYS:NZ	1:A:147:GLN:OE1	2.54	0.41
1:B:27:THR:HG22	1:B:202:VAL:HG13	2.03	0.41
2:C:230:PHE:HE1	2:C:287:VAL:HG21	1.85	0.41
2:C:560:PRO:HB2	3:D:776:THR:HG21	2.03	0.41
3:D:128:LEU:HA	3:D:192:MET:HE1	2.03	0.41
3:D:573:THR:OG1	3:D:576:ARG:HG3	2.20	0.41
3:D:853:THR:HG22	3:D:854:ALA:H	1.86	0.41
5:F:559:LEU:O	5:F:563:PHE:HD2	2.03	0.41
1:G:93:GLN:HB2	1:G:120:ASP:OD2	2.21	0.41
1:H:102:LEU:HD23	1:H:115:ILE:HG23	2.02	0.41
1:H:29:GLU:HB3	1:H:30:PRO:CD	2.48	0.41
2:I:409:LEU:HD23	2:I:409:LEU:HA	1.93	0.41
3:J:579:LEU:HD12	3:J:582:ILE:HD12	2.01	0.41
1:B:16:ILE:HG13	1:B:26:VAL:HG22	2.03	0.40
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.56	0.40
2:C:37:LYS:HA	2:C:37:LYS:HD3	1.79	0.40
2:C:65:ASN:HB3	2:C:105:TYR:HB2	2.03	0.40
2:C:732:ILE:HD11	2:C:769:PRO:HB3	2.03	0.40
3:D:197:GLU:O	3:D:201:LEU:HG	2.21	0.40
3:D:572:THR:OG1	3:D:573:THR:N	2.54	0.40
5:F:482:GLU:HG2	5:F:486:ARG:HH22	1.86	0.40
5:F:511:ILE:HA	5:F:511:ILE:HD12	1.86	0.40
6:I:2001:4OB:H7	3:J:774:ILE:HG13	2.02	0.40
2:I:468:LEU:HA	2:I:471:VAL:HG12	2.03	0.40
2:I:561:ILE:HD11	2:I:665:ALA:HB1	2.02	0.40
2:I:80:PHE:HB2	2:I:85:CYS:SG	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:867:GLU:HG3	2:I:867:GLU:H	1.65	0.40
2:I:972:PHE:CD2	2:I:975:ILE:HD12	2.56	0.40
2:I:1287:LEU:HD22	3:J:1357:ILE:HD11	2.03	0.40
3:J:128:LEU:HA	3:J:192:MET:HE1	2.03	0.40
3:J:505:ASP:HB2	3:J:629:PHE:HE1	1.87	0.40
3:J:740:LEU:HA	3:J:740:LEU:HD12	1.91	0.40
5:L:22:LEU:H	5:L:54:GLN:CB	2.34	0.40
5:L:29:ASP:OD1	5:L:30:HIS:N	2.54	0.40
5:L:348:GLU:HG2	5:L:354:THR:HA	2.04	0.40
5:L:484:ALA:HB1	5:L:491:GLU:HB2	2.02	0.40
2:C:163:LYS:HB3	2:C:163:LYS:HE3	1.89	0.40
2:C:356:THR:HG21	2:C:362:ALA:HA	2.03	0.40
3:D:657:ALA:O	3:D:661:VAL:HG13	2.21	0.40
1:G:145:LYS:NZ	1:G:147:GLN:OE1	2.54	0.40
1:G:51:MET:HB3	1:G:51:MET:HE3	1.93	0.40
2:I:130:MET:HB2	2:I:136:PHE:CZ	2.56	0.40
2:I:721:GLY:N	2:I:740:GLU:OE1	2.50	0.40
3:J:37:GLU:HB2	3:J:104:HIS:CE1	2.56	0.40
3:J:708:ASN:HB3	3:J:712:GLN:O	2.21	0.40
5:L:362:ASN:HB2	5:L:365:MET:HE2	2.03	0.40
3:J:291:ILE:HD13	5:L:409:ASN:HB3	2.03	0.40
2:C:35:PHE:CD2	2:C:130:MET:HB3	2.57	0.40
2:C:484:LEU:HD12	2:C:485:ASP:H	1.86	0.40
2:C:552:PRO:HG3	6:C:2001:4OB:CAL	2.51	0.40
5:F:399:LEU:HA	5:F:399:LEU:HD12	1.86	0.40
5:F:465:ARG:HA	5:F:468:ARG:HH12	1.86	0.40
1:G:162:GLU:HB3	1:G:163:GLU:H	1.72	0.40
1:G:92:VAL:HA	1:G:120:ASP:O	2.21	0.40
1:H:33:ARG:NH1	2:I:1081:PRO:HG3	2.32	0.40
2:I:466:VAL:O	2:I:469:VAL:HG22	2.21	0.40
2:I:521:LEU:HD23	2:I:708:VAL:HG11	2.03	0.40
2:I:658:GLN:O	2:I:660:VAL:N	2.54	0.40
2:I:813:GLU:HB2	3:J:461:PHE:HB2	2.03	0.40
2:I:959:ASP:O	2:I:963:GLU:HG2	2.21	0.40
3:J:233:LYS:HA	3:J:234:PRO:HD3	1.93	0.40
3:J:682:VAL:HA	3:J:685:ILE:CD1	2.52	0.40
5:L:354:THR:O	5:L:358:VAL:HG23	2.21	0.40
1:B:65:LEU:HD13	1:B:65:LEU:O	2.22	0.40
2:C:930:ASP:HB3	2:C:1053:TYR:HB2	2.03	0.40
2:C:1253:LEU:O	3:D:99:ARG:NH2	2.55	0.40
2:C:498:ILE:HD12	2:C:498:ILE:H	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:521:LEU:HD23	2:C:708:VAL:HG11	2.03	0.40
2:C:557:ARG:HH21	2:C:607:SER:C	2.24	0.40
3:D:756:GLU:H	3:D:756:GLU:HG2	1.57	0.40
3:D:870:ASP:O	3:D:874:GLU:HG2	2.21	0.40
3:D:901:ARG:HA	3:D:908:ILE:HA	2.02	0.40
2:I:1179:GLY:O	2:I:1181:PRO:HD3	2.21	0.40
2:I:967:LEU:HA	2:I:967:LEU:HD12	1.93	0.40
3:J:97:VAL:HG12	3:J:101:ARG:HG3	2.04	0.40
3:J:1061:VAL:HG21	3:J:1101:LEU:HB2	2.03	0.40
3:J:969:SER:HB3	3:J:1116:SER:HB2	2.03	0.40
3:J:34:SER:HG	3:J:104:HIS:CG	2.29	0.40
3:J:706:VAL:HG12	3:J:715:LYS:HB3	2.04	0.40
3:J:905:ARG:NH1	4:K:16:ARG:HD2	2.26	0.40
3:D:1162:ILE:HA	3:D:1203:ARG:HA	2.04	0.40
3:D:1368:ASP:OD1	3:D:1371:ARG:NH2	2.55	0.40
3:D:905:ARG:HE	3:D:907:HIS:HB2	1.86	0.40
5:F:348:GLU:HG2	5:F:354:THR:HA	2.03	0.40
1:H:112:ALA:HB2	1:H:128:HIS:HB3	2.02	0.40
3:J:1031:VAL:HG23	3:J:1080:ILE:HG21	2.04	0.40
3:J:1194:ARG:HD2	3:J:1194:ARG:N	2.36	0.40
3:J:925:GLU:HB3	3:J:926:PRO:HD3	2.03	0.40
5:L:561:MET:HG3	5:L:571:TYR:HD2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	298/335 (89%)	270 (91%)	19 (6%)	9 (3%)	4	32
1	B	212/335 (63%)	190 (90%)	20 (9%)	2 (1%)	17	56
1	G	222/335 (66%)	196 (88%)	20 (9%)	6 (3%)	5	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	212/335 (63%)	193 (91%)	17 (8%)	2 (1%)	17	56
2	C	1338/1342 (100%)	1234 (92%)	98 (7%)	6 (0%)	34	72
2	I	1338/1342 (100%)	1232 (92%)	100 (8%)	6 (0%)	34	72
3	D	1162/1407 (83%)	1045 (90%)	105 (9%)	12 (1%)	15	54
3	J	1328/1407 (94%)	1195 (90%)	122 (9%)	11 (1%)	19	60
4	E	87/91 (96%)	81 (93%)	6 (7%)	0	100	100
4	K	77/91 (85%)	73 (95%)	4 (5%)	0	100	100
5	F	532/613 (87%)	481 (90%)	50 (9%)	1 (0%)	47	81
5	L	529/613 (86%)	480 (91%)	49 (9%)	0	100	100
All	All	7335/8246 (89%)	6670 (91%)	610 (8%)	55 (1%)	22	62

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	GLU
1	A	320	ASN
2	C	237	LEU
3	D	120	LEU
3	D	751	ASP
2	I	237	LEU
3	J	120	LEU
3	J	751	ASP
1	A	193	GLU
1	A	323	PRO
1	B	15	ASP
2	C	170	VAL
3	D	10	ALA
3	D	89	GLY
3	D	753	SER
1	G	193	GLU
2	I	170	VAL
3	J	89	GLY
3	J	753	SER
1	A	62	ASP
3	D	756	GLU
5	F	7	SER
1	G	62	ASP
3	J	756	GLU
1	A	196	THR

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Mol	Chain	Res	Type
2	C	1136	GLN
3	D	710	ASP
1	G	196	THR
1	G	229	GLU
1	H	29	GLU
2	I	1136	GLN
3	J	710	ASP
1	A	167	PRO
2	C	697	LYS
3	D	777	HIS
1	G	167	PRO
1	G	178	SER
2	I	697	LYS
1	A	178	SER
1	B	193	GLU
2	C	1186	VAL
3	D	778	GLY
3	D	831	VAL
1	H	193	GLU
2	I	1186	VAL
3	J	831	VAL
3	D	758	PRO
3	J	749	LYS
3	J	778	GLY
3	J	758	PRO
1	A	14	VAL
2	C	1159	VAL
3	D	749	LYS
2	I	1159	VAL
3	J	752	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	257/292 (88%)	241 (94%)	16 (6%)	18 46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	184/292 (63%)	168 (91%)	16 (9%)	10	34
1	G	191/292 (65%)	182 (95%)	9 (5%)	26	53
1	H	183/292 (63%)	171 (93%)	12 (7%)	16	44
2	C	1155/1157 (100%)	1065 (92%)	90 (8%)	12	39
2	I	1154/1157 (100%)	1060 (92%)	94 (8%)	11	38
3	D	975/1168 (84%)	886 (91%)	89 (9%)	9	32
3	J	1117/1168 (96%)	1019 (91%)	98 (9%)	10	34
4	E	72/75 (96%)	66 (92%)	6 (8%)	11	37
4	K	67/75 (89%)	61 (91%)	6 (9%)	9	33
5	F	426/540 (79%)	392 (92%)	34 (8%)	12	38
5	L	428/540 (79%)	393 (92%)	35 (8%)	11	37
All	All	6209/7048 (88%)	5704 (92%)	505 (8%)	11	38

All (505) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	10	LYS
1	A	13	LEU
1	A	35	PHE
1	A	54	CYS
1	A	133	LEU
1	A	145	LYS
1	A	148	ARG
1	A	186	ASN
1	A	207	THR
1	A	215	GLU
1	A	287	VAL
1	A	317	ARG
1	A	318	LEU
1	A	319	GLU
1	A	321	TRP
1	B	8	PHE
1	B	9	LEU
1	B	14	VAL
1	B	29	GLU
1	B	31	LEU
1	B	54	CYS

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Mol	Chain	Res	Type
1	B	60	GLU
1	B	75	GLN
1	B	79	LEU
1	B	101	THR
1	B	105	SER
1	B	116	THR
1	B	133	LEU
1	B	160	HIS
1	B	183	ILE
1	B	186	ASN
2	C	11	ILE
2	C	29	SER
2	C	39	ILE
2	C	70	TYR
2	C	81	ASP
2	C	85	CYS
2	C	91	THR
2	C	115	LYS
2	C	116	ASP
2	C	119	GLU
2	C	131	THR
2	C	179	TYR
2	C	182	SER
2	C	185	ASP
2	C	202	ARG
2	C	285	ILE
2	C	320	ASP
2	C	321	LEU
2	C	419	ILE
2	C	423	ASP
2	C	434	ASP
2	C	484	LEU
2	C	485	ASP
2	C	486	THR
2	C	487	LEU
2	C	493	ILE
2	C	512	SER
2	C	517	GLN
2	C	518	ASN
2	C	530	ILE
2	C	538	LEU
2	C	539	THR

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Mol	Chain	Res	Type
2	C	540	ARG
2	C	554	HIS
2	C	604	HIS
2	C	615	VAL
2	C	618	GLN
2	C	623	LEU
2	C	633	LEU
2	C	657	THR
2	C	672	GLU
2	C	692	THR
2	C	697	LYS
2	C	699	LEU
2	C	706	ARG
2	C	714	VAL
2	C	739	ASP
2	C	748	ILE
2	C	765	ILE
2	C	773	LEU
2	C	781	ASP
2	C	788	SER
2	C	815	SER
2	C	819	SER
2	C	828	PHE
2	C	839	VAL
2	C	859	GLU
2	C	878	THR
2	C	890	LYS
2	C	892	GLU
2	C	895	LEU
2	C	974	ARG
2	C	990	ASP
2	C	992	LEU
2	C	1002	LEU
2	C	1005	GLU
2	C	1006	GLU
2	C	1014	LEU
2	C	1040	ASP
2	C	1082	ILE
2	C	1108	ASN
2	C	1109	ILE
2	C	1114	GLU
2	C	1134	GLN

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Mol	Chain	Res	Type
2	C	1155	VAL
2	C	1156	ARG
2	C	1161	LEU
2	C	1198	LEU
2	C	1204	LEU
2	C	1210	ILE
2	C	1237	HIS
2	C	1240	ASP
2	C	1248	THR
2	C	1264	GLN
2	C	1265	PHE
2	C	1310	ASP
2	C	1313	HIS
2	C	1326	LEU
2	C	1327	LEU
2	C	1342	GLU
3	D	8	LEU
3	D	11	GLN
3	D	18	ASP
3	D	20	ILE
3	D	46	TYR
3	D	79	LYS
3	D	88	CYS
3	D	92	VAL
3	D	95	THR
3	D	117	LEU
3	D	119	SER
3	D	120	LEU
3	D	169	LEU
3	D	175	GLU
3	D	176	PHE
3	D	217	LEU
3	D	248	ASP
3	D	252	LEU
3	D	255	LEU
3	D	256	ASP
3	D	264	ASP
3	D	311	ARG
3	D	324	LEU
3	D	339	ARG
3	D	356	THR
3	D	364	HIS

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Mol	Chain	Res	Type
3	D	374	LEU
3	D	430	HIS
3	D	474	LEU
3	D	506	VAL
3	D	536	LEU
3	D	545	HIS
3	D	547	ARG
3	D	568	SER
3	D	593	ASN
3	D	594	GLN
3	D	641	ILE
3	D	660	GLU
3	D	678	ARG
3	D	683	ILE
3	D	697	MET
3	D	698	MET
3	D	701	LEU
3	D	707	ILE
3	D	708	ASN
3	D	710	ASP
3	D	712	GLN
3	D	717	VAL
3	D	740	LEU
3	D	746	LEU
3	D	749	LYS
3	D	754	ILE
3	D	756	GLU
3	D	760	THR
3	D	764	ARG
3	D	767	LEU
3	D	810	THR
3	D	847	ASP
3	D	848	VAL
3	D	849	LEU
3	D	853	THR
3	D	857	LEU
3	D	860	ARG
3	D	867	GLN
3	D	897	HIS
3	D	908	ILE
3	D	918	ILE
3	D	928	THR

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Mol	Chain	Res	Type
3	D	931	THR
3	D	1155	ILE
3	D	1163	VAL
3	D	1167	LYS
3	D	1173	ARG
3	D	1177	ILE
3	D	1186	TYR
3	D	1199	PHE
3	D	1202	GLU
3	D	1208	ASP
3	D	1209	VAL
3	D	1215	GLU
3	D	1244	GLN
3	D	1274	PHE
3	D	1275	LEU
3	D	1281	GLU
3	D	1284	ARG
3	D	1289	ASN
3	D	1293	GLU
3	D	1327	GLU
3	D	1333	THR
4	E	28	ARG
4	E	31	GLN
4	E	36	ASP
4	E	39	VAL
4	E	46	THR
4	E	58	LEU
5	F	27	VAL
5	F	44	ILE
5	F	45	ILE
5	F	50	ASP
5	F	98	VAL
5	F	100	MET
5	F	118	ASP
5	F	154	GLU
5	F	305	LEU
5	F	306	PHE
5	F	341	LEU
5	F	395	THR
5	F	417	ASP
5	F	421	TYR
5	F	429	THR

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Mol	Chain	Res	Type
5	F	445	ASP
5	F	449	THR
5	F	479	THR
5	F	486	ARG
5	F	488	LEU
5	F	491	GLU
5	F	496	LYS
5	F	508	GLU
5	F	528	LEU
5	F	530	LEU
5	F	540	LEU
5	F	566	ASP
5	F	568	ASN
5	F	572	THR
5	F	573	LEU
5	F	580	PHE
5	F	583	THR
5	F	600	HIS
5	F	606	VAL
1	G	9	LEU
1	G	13	LEU
1	G	35	PHE
1	G	54	CYS
1	G	133	LEU
1	G	145	LYS
1	G	186	ASN
1	G	207	THR
1	G	215	GLU
1	H	13	LEU
1	H	28	LEU
1	H	31	LEU
1	H	54	CYS
1	H	60	GLU
1	H	75	GLN
1	H	79	LEU
1	H	101	THR
1	H	116	THR
1	H	133	LEU
1	H	183	ILE
1	H	186	ASN
2	I	11	ILE
2	I	29	SER

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Mol	Chain	Res	Type
2	I	39	ILE
2	I	70	TYR
2	I	81	ASP
2	I	85	CYS
2	I	91	THR
2	I	115	LYS
2	I	116	ASP
2	I	119	GLU
2	I	131	THR
2	I	179	TYR
2	I	182	SER
2	I	185	ASP
2	I	202	ARG
2	I	219	GLN
2	I	285	ILE
2	I	320	ASP
2	I	321	LEU
2	I	419	ILE
2	I	423	ASP
2	I	434	ASP
2	I	484	LEU
2	I	485	ASP
2	I	486	THR
2	I	487	LEU
2	I	493	ILE
2	I	512	SER
2	I	517	GLN
2	I	518	ASN
2	I	530	ILE
2	I	538	LEU
2	I	539	THR
2	I	540	ARG
2	I	554	HIS
2	I	604	HIS
2	I	615	VAL
2	I	618	GLN
2	I	623	LEU
2	I	633	LEU
2	I	641	GLU
2	I	657	THR
2	I	672	GLU
2	I	692	THR

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Mol	Chain	Res	Type
2	I	697	LYS
2	I	699	LEU
2	I	706	ARG
2	I	714	VAL
2	I	739	ASP
2	I	748	ILE
2	I	765	ILE
2	I	773	LEU
2	I	781	ASP
2	I	782	VAL
2	I	788	SER
2	I	815	SER
2	I	819	SER
2	I	828	PHE
2	I	839	VAL
2	I	859	GLU
2	I	878	THR
2	I	890	LYS
2	I	892	GLU
2	I	895	LEU
2	I	974	ARG
2	I	990	ASP
2	I	992	LEU
2	I	1002	LEU
2	I	1005	GLU
2	I	1006	GLU
2	I	1014	LEU
2	I	1040	ASP
2	I	1082	ILE
2	I	1108	ASN
2	I	1109	ILE
2	I	1114	GLU
2	I	1134	GLN
2	I	1155	VAL
2	I	1156	ARG
2	I	1158	LYS
2	I	1161	LEU
2	I	1198	LEU
2	I	1204	LEU
2	I	1210	ILE
2	I	1237	HIS
2	I	1240	ASP

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Mol	Chain	Res	Type
2	I	1248	THR
2	I	1264	GLN
2	I	1265	PHE
2	I	1310	ASP
2	I	1313	HIS
2	I	1326	LEU
2	I	1327	LEU
2	I	1342	GLU
3	J	18	ASP
3	J	20	ILE
3	J	46	TYR
3	J	79	LYS
3	J	88	CYS
3	J	92	VAL
3	J	95	THR
3	J	117	LEU
3	J	119	SER
3	J	120	LEU
3	J	169	LEU
3	J	175	GLU
3	J	176	PHE
3	J	217	LEU
3	J	248	ASP
3	J	252	LEU
3	J	255	LEU
3	J	256	ASP
3	J	264	ASP
3	J	311	ARG
3	J	324	LEU
3	J	339	ARG
3	J	356	THR
3	J	364	HIS
3	J	374	LEU
3	J	430	HIS
3	J	474	LEU
3	J	506	VAL
3	J	545	HIS
3	J	547	ARG
3	J	568	SER
3	J	593	ASN
3	J	594	GLN
3	J	641	ILE

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Mol	Chain	Res	Type
3	J	660	GLU
3	J	678	ARG
3	J	683	ILE
3	J	697	MET
3	J	698	MET
3	J	701	LEU
3	J	707	ILE
3	J	708	ASN
3	J	710	ASP
3	J	712	GLN
3	J	717	VAL
3	J	740	LEU
3	J	746	LEU
3	J	749	LYS
3	J	754	ILE
3	J	756	GLU
3	J	760	THR
3	J	764	ARG
3	J	767	LEU
3	J	772	TYR
3	J	773	PHE
3	J	788	LEU
3	J	810	THR
3	J	847	ASP
3	J	848	VAL
3	J	849	LEU
3	J	853	THR
3	J	857	LEU
3	J	860	ARG
3	J	867	GLN
3	J	897	HIS
3	J	908	ILE
3	J	918	ILE
3	J	928	THR
3	J	931	THR
3	J	987	GLU
3	J	997	VAL
3	J	1017	VAL
3	J	1025	MET
3	J	1042	ASP
3	J	1062	LEU
3	J	1063	ASP

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Mol	Chain	Res	Type
3	J	1073	ASP
3	J	1115	ILE
3	J	1155	ILE
3	J	1163	VAL
3	J	1167	LYS
3	J	1173	ARG
3	J	1177	ILE
3	J	1186	TYR
3	J	1199	PHE
3	J	1202	GLU
3	J	1208	ASP
3	J	1209	VAL
3	J	1215	GLU
3	J	1244	GLN
3	J	1274	PHE
3	J	1275	LEU
3	J	1281	GLU
3	J	1284	ARG
3	J	1289	ASN
3	J	1293	GLU
3	J	1327	GLU
3	J	1333	THR
4	K	28	ARG
4	K	31	GLN
4	K	36	ASP
4	K	39	VAL
4	K	46	THR
4	K	58	LEU
5	L	27	VAL
5	L	44	ILE
5	L	45	ILE
5	L	50	ASP
5	L	98	VAL
5	L	100	MET
5	L	118	ASP
5	L	127	ILE
5	L	154	GLU
5	L	244	THR
5	L	305	LEU
5	L	306	PHE
5	L	335	GLU
5	L	341	LEU

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Mol	Chain	Res	Type
5	L	395	THR
5	L	417	ASP
5	L	421	TYR
5	L	445	ASP
5	L	449	THR
5	L	479	THR
5	L	486	ARG
5	L	488	LEU
5	L	491	GLU
5	L	496	LYS
5	L	508	GLU
5	L	528	LEU
5	L	530	LEU
5	L	540	LEU
5	L	566	ASP
5	L	568	ASN
5	L	572	THR
5	L	573	LEU
5	L	580	PHE
5	L	583	THR
5	L	600	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	GLN
1	A	320	ASN
2	C	343	HIS
2	C	1108	ASN
2	C	1111	GLN
2	C	1116	HIS
2	C	1288	GLN
2	C	1314	GLN
3	D	340	GLN
3	D	364	HIS
3	D	419	HIS
3	D	560	ASN
3	D	1367	GLN
5	F	406	GLN
5	F	600	HIS
2	I	343	HIS
2	I	357	ASN

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Mol	Chain	Res	Type
2	I	1108	ASN
2	I	1111	GLN
2	I	1116	HIS
2	I	1257	GLN
2	I	1314	GLN
3	J	340	GLN
3	J	364	HIS
3	J	419	HIS
3	J	560	ASN
3	J	1367	GLN
5	L	406	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	4OB	I	2001	-	21,21,21	2.41	5 (23%)	28,29,29	1.43	5 (17%)
6	4OB	C	2001	-	21,21,21	2.41	5 (23%)	28,29,29	1.43	5 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	4OB	I	2001	-	-	1/15/16/16	0/2/2/2
6	4OB	C	2001	-	-	1/15/16/16	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	2001	4OB	CAQ-NAO	-6.57	1.31	1.42
6	C	2001	4OB	CAQ-NAO	-6.56	1.31	1.42
6	I	2001	4OB	CAT-CAS	-5.97	1.37	1.49
6	C	2001	4OB	CAT-CAS	-5.96	1.37	1.49
6	C	2001	4OB	CAR-CAP	-4.53	1.39	1.47
6	I	2001	4OB	CAR-CAP	-4.52	1.39	1.47
6	C	2001	4OB	CAP-NAO	3.20	1.33	1.28
6	I	2001	4OB	CAP-NAO	3.18	1.33	1.28
6	I	2001	4OB	OAA-NAN	2.96	1.47	1.40
6	C	2001	4OB	OAA-NAN	2.96	1.47	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	2001	4OB	CAM-CAS-CAT	3.19	123.89	119.58
6	C	2001	4OB	CAM-CAS-CAT	3.17	123.87	119.58
6	I	2001	4OB	CAL-CAS-CAT	-2.77	115.56	119.97
6	C	2001	4OB	CAL-CAS-CAT	-2.77	115.57	119.97
6	C	2001	4OB	OAA-NAN-CAP	-2.58	113.26	119.49
6	I	2001	4OB	OAA-NAN-CAP	-2.57	113.29	119.49
6	I	2001	4OB	CAK-CAR-CAP	-2.36	116.69	120.86
6	C	2001	4OB	CAK-CAR-CAP	-2.36	116.69	120.86
6	C	2001	4OB	CAQ-NAO-CAP	2.35	125.52	120.41
6	I	2001	4OB	CAQ-NAO-CAP	2.34	125.50	120.41

There are no chirality outliers.

All (2) torsion outliers are listed below:

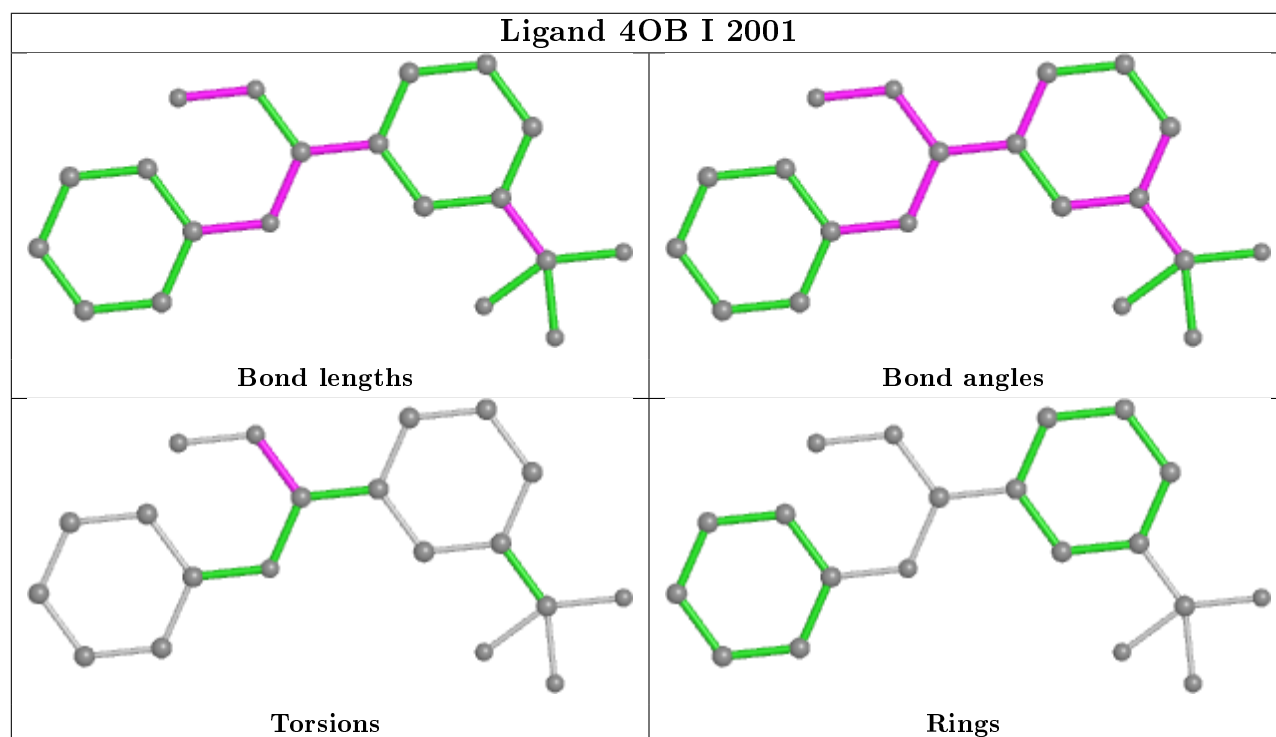
Mol	Chain	Res	Type	Atoms
6	I	2001	4OB	CAR-CAP-NAN-OAA
6	C	2001	4OB	CAR-CAP-NAN-OAA

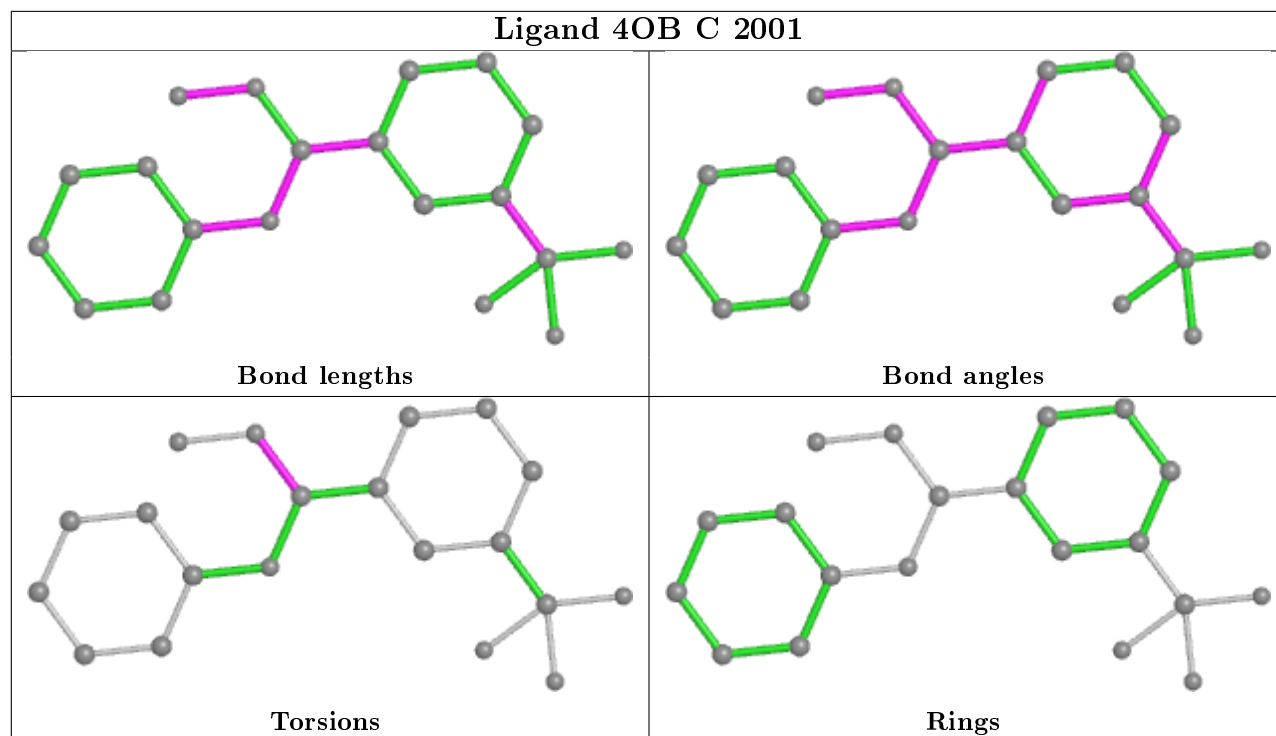
There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	2001	4OB	8	0
6	C	2001	4OB	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	302/335 (90%)	-0.03	7 (2%) 60 51	28, 105, 237, 409	0
1	B	216/335 (64%)	-0.14	7 (3%) 47 37	28, 127, 210, 290	0
1	G	224/335 (66%)	-0.03	4 (1%) 68 59	59, 127, 200, 244	0
1	H	216/335 (64%)	0.13	8 (3%) 41 33	49, 145, 220, 274	0
2	C	1340/1342 (99%)	-0.13	26 (1%) 66 58	15, 95, 231, 320	0
2	I	1340/1342 (99%)	0.07	59 (4%) 34 28	21, 132, 241, 336	0
3	D	1166/1407 (82%)	-0.18	11 (0%) 84 77	13, 70, 178, 278	0
3	J	1334/1407 (94%)	-0.01	44 (3%) 46 37	16, 95, 214, 287	0
4	E	89/91 (97%)	-0.33	0 100 100	16, 93, 132, 215	0
4	K	79/91 (86%)	-0.13	0 100 100	54, 120, 204, 224	0
5	F	542/613 (88%)	0.18	35 (6%) 18 15	31, 145, 251, 341	0
5	L	539/613 (87%)	0.17	39 (7%) 15 13	34, 147, 248, 314	0
All	All	7387/8246 (89%)	-0.02	240 (3%) 47 37	13, 110, 229, 409	0

All (240) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	74	GLU	10.1
5	L	8	GLN	7.2
5	F	88	GLU	7.1
3	J	1054	THR	7.1
5	F	89	SER	7.0
5	L	30	HIS	6.7
5	F	75	ASP	6.4
3	J	1068	THR	6.0
5	L	39	ASP	5.9
5	L	38	SER	5.9
5	L	37	ASP	5.9

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Mol	Chain	Res	Type	RSRZ
5	F	73	ASP	5.7
5	F	33	GLU	5.6
3	J	1069	ALA	5.4
2	I	982	GLY	5.2
2	C	291	TYR	5.2
5	L	10	LYS	5.1
2	I	989	LEU	5.1
3	J	1055	GLY	4.9
5	F	86	SER	4.9
5	F	34	ASP	4.8
5	L	43	ASP	4.7
5	F	76	ALA	4.7
2	C	252	SER	4.7
5	L	18	GLU	4.7
5	L	49	ASN	4.6
1	B	69	SER	4.5
2	I	251	ALA	4.5
2	I	973	SER	4.5
3	J	1161	GLY	4.5
5	L	50	ASP	4.4
3	J	518	VAL	4.4
2	C	292	ILE	4.4
5	F	579	GLN	4.3
5	L	40	GLN	4.3
2	I	988	LYS	4.3
3	J	1071	GLY	4.2
3	J	955	LYS	4.2
2	I	978	VAL	4.2
2	C	312	ALA	4.2
5	F	32	PRO	4.1
2	C	311	CYS	4.1
2	C	374	GLU	4.1
3	J	1070	GLY	4.1
2	C	265	LYS	4.0
5	F	575	GLU	3.9
5	L	7	SER	3.9
3	J	1056	LEU	3.9
2	I	305	SER	3.9
2	I	999	GLU	3.9
1	B	67	GLU	3.9
5	L	29	ASP	3.8
3	D	1161	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	172	LEU	3.8
2	I	322	LEU	3.7
5	F	167	ASP	3.7
5	L	32	PRO	3.6
5	L	47	MET	3.6
2	I	981	ALA	3.6
3	J	1160	SER	3.6
2	I	976	ARG	3.6
2	I	231	GLU	3.6
5	F	87	VAL	3.6
5	L	9	LEU	3.6
5	L	11	LEU	3.6
2	I	317	LEU	3.5
5	F	85	SER	3.5
3	D	826	ILE	3.5
3	J	974	VAL	3.5
2	C	314	ASN	3.5
5	L	167	ASP	3.5
2	I	229	ILE	3.4
5	L	34	ASP	3.4
2	I	974	ARG	3.4
2	I	882	ILE	3.3
1	B	68	TYR	3.3
2	I	986	ALA	3.3
2	I	267	ARG	3.3
3	J	1115	ILE	3.3
2	I	975	ILE	3.2
1	H	172	LEU	3.2
2	C	107	ARG	3.1
3	D	678	ARG	3.1
3	D	1203	ARG	3.1
3	J	1051	ASP	3.1
2	I	969	ALA	3.1
2	I	1021	LEU	3.1
5	L	41	ILE	3.1
5	L	305	LEU	3.0
2	C	373	GLY	3.0
2	I	726	TYR	3.0
1	A	266	SER	3.0
1	B	158	ARG	3.0
2	I	979	LEU	3.0
2	I	334	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	146	VAL	2.9
2	I	743	PRO	2.9
3	J	1013	GLY	2.9
3	J	1012	ALA	2.9
2	I	990	ASP	2.9
2	I	1020	GLU	2.8
3	J	1114	GLN	2.8
2	I	725	GLN	2.8
1	H	97	GLU	2.8
3	J	975	ILE	2.8
3	J	1036	ARG	2.8
2	C	283	LYS	2.7
3	J	1094	ASP	2.7
2	I	1005	GLU	2.7
5	L	46	GLN	2.7
2	C	305	SER	2.7
2	C	338	THR	2.7
2	I	120	GLN	2.7
2	I	311	CYS	2.7
3	J	1073	ASP	2.7
5	F	9	LEU	2.7
2	I	333	ILE	2.6
3	J	989	GLY	2.6
5	L	31	LEU	2.6
3	J	1188	GLU	2.6
5	F	584	ARG	2.6
5	F	283	GLN	2.6
5	L	86	SER	2.6
2	I	169	LYS	2.6
2	I	304	GLU	2.6
1	H	90	VAL	2.6
3	J	1152	GLU	2.6
5	F	318	ALA	2.6
2	I	970	GLY	2.6
1	H	146	VAL	2.5
2	I	332	ARG	2.5
5	F	319	ALA	2.5
1	A	270	LEU	2.5
5	F	421	TYR	2.5
2	C	317	LEU	2.5
2	I	264	GLU	2.5
3	D	1165	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	90	VAL	2.5
3	J	1053	LEU	2.5
3	J	1065	ALA	2.5
2	I	987	GLU	2.5
1	A	262	LEU	2.5
5	L	488	LEU	2.5
5	F	256	PHE	2.5
2	C	56	VAL	2.4
2	I	234	ASP	2.4
2	C	251	ALA	2.4
1	A	264	VAL	2.4
1	H	92	VAL	2.4
3	J	648	GLU	2.4
3	J	986	ASP	2.4
5	L	24	TYR	2.4
2	I	443	ASP	2.4
5	L	85	SER	2.4
5	F	578	LYS	2.4
2	C	313	ALA	2.4
2	C	68	LEU	2.4
2	I	230	PHE	2.4
3	J	966	VAL	2.4
2	C	350	THR	2.4
2	I	420	LEU	2.3
1	G	21	SER	2.3
3	J	988	PHE	2.3
1	A	267	ALA	2.3
3	D	682	VAL	2.3
3	J	674	THR	2.3
5	F	8	GLN	2.3
5	L	82	GLN	2.3
2	I	626	GLU	2.3
3	J	1186	TYR	2.3
2	C	1001	GLY	2.3
5	L	25	ALA	2.3
5	L	286	LEU	2.3
5	L	48	ILE	2.3
5	F	259	PHE	2.3
2	I	295	LYS	2.3
5	L	42	GLU	2.3
2	I	233	ARG	2.3
5	F	27	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	I	1004	ASP	2.3
2	I	985	GLU	2.3
3	D	830	ASP	2.3
5	F	19	GLN	2.3
3	J	1087	ASP	2.2
5	L	33	GLU	2.2
2	C	288	PRO	2.2
3	J	647	PRO	2.2
1	H	59	VAL	2.2
3	J	392	THR	2.2
2	I	203	LYS	2.2
3	J	76	LYS	2.2
2	C	205	PRO	2.2
2	I	727	VAL	2.2
3	D	1180	VAL	2.2
3	D	1204	VAL	2.2
2	C	100	LEU	2.2
5	F	162	ILE	2.2
3	J	991	THR	2.2
5	L	89	SER	2.2
2	I	1002	LEU	2.2
2	I	1160	ASP	2.2
3	J	1095	MET	2.2
5	F	72	ALA	2.2
5	F	158	LEU	2.2
3	J	744	ARG	2.2
2	I	258	ASN	2.2
2	I	100	LEU	2.1
3	J	317	THR	2.1
2	I	292	ILE	2.1
5	L	70	ASN	2.1
3	J	1108	GLN	2.1
5	L	14	THR	2.1
3	J	954	ASN	2.1
2	C	66	SER	2.1
5	F	77	ALA	2.1
1	A	263	THR	2.1
2	C	59	ILE	2.1
2	I	634	VAL	2.1
1	H	67	GLU	2.1
3	D	674	THR	2.1
5	F	140	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	I	80	PHE	2.1
5	F	165	PHE	2.1
1	G	54	CYS	2.1
2	I	318	SER	2.1
5	F	137	TYR	2.1
5	L	165	PHE	2.1
3	J	1215	GLU	2.1
1	H	52	PRO	2.1
2	C	287	VAL	2.1
2	I	243	PRO	2.1
5	F	490	PRO	2.1
5	L	87	VAL	2.1
3	J	1151	LYS	2.0
5	L	84	LEU	2.0
3	D	1171	GLY	2.0
1	B	78	ILE	2.0
1	G	213	PRO	2.0
2	I	291	TYR	2.0
1	A	271	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	4OB	I	2001	20/20	0.74	0.92	90,112,127,136	0
6	4OB	C	2001	20/20	0.83	0.75	50,73,98,99	0
7	MG	D	1501	1/1	0.86	0.80	72,72,72,72	0
8	ZN	D	1502	1/1	0.93	0.10	90,90,90,90	0

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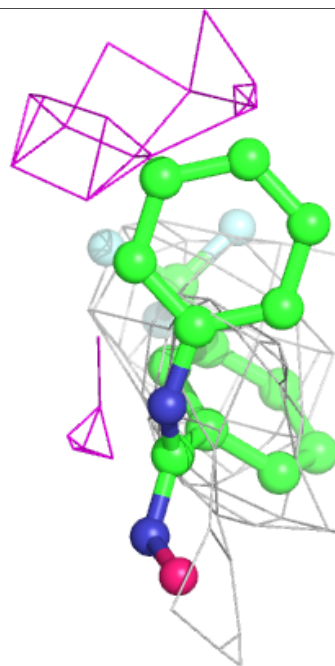
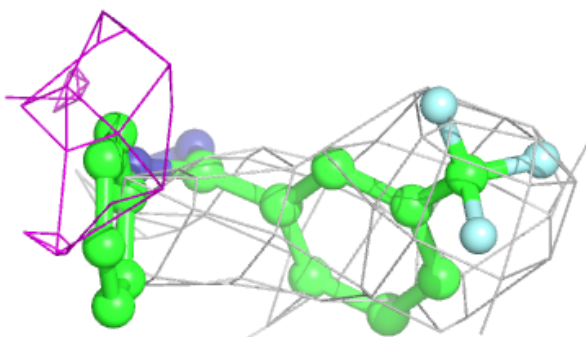
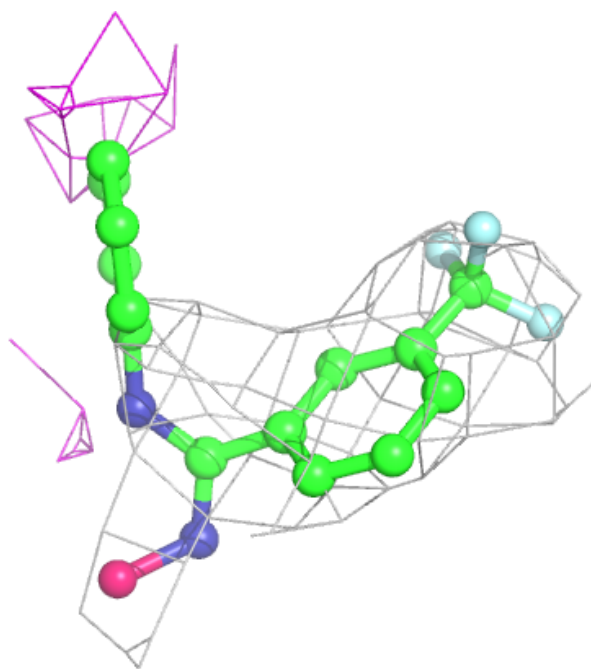
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	ZN	D	1503	1/1	0.94	0.39	138,138,138,138	0
8	ZN	J	1502	1/1	0.95	0.13	79,79,79,79	0
7	MG	J	1501	1/1	0.96	0.69	33,33,33,33	0
8	ZN	J	1503	1/1	0.98	0.20	31,31,31,31	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

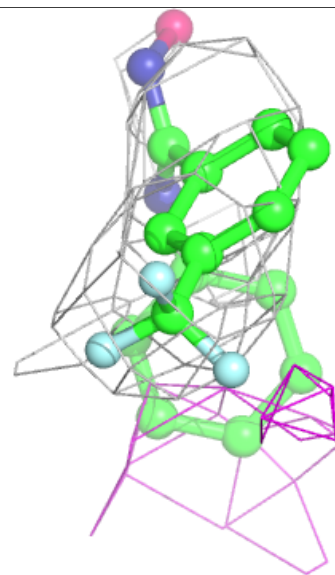
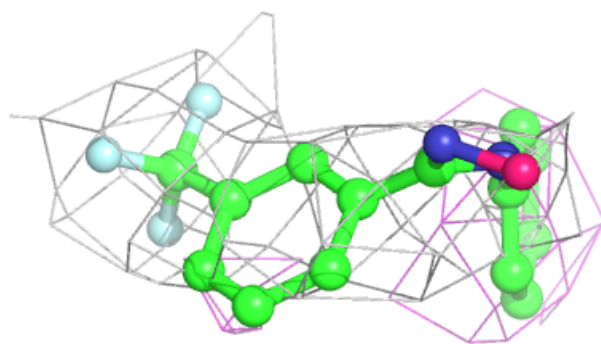
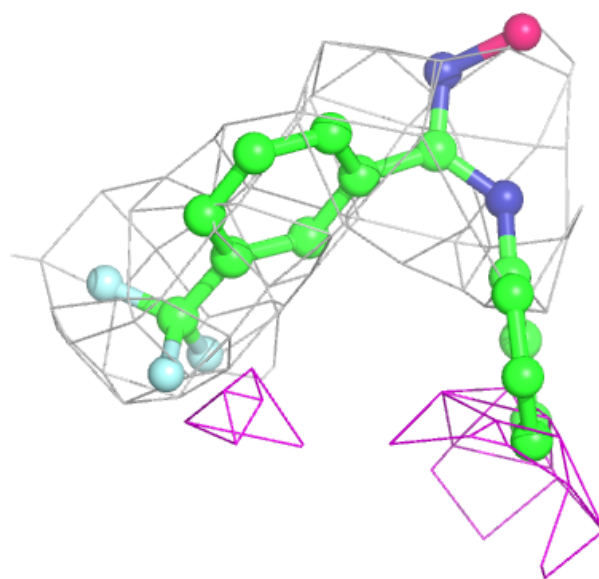
Electron density around 4OB I 2001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 4OB C 2001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.